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TECHNICAL ABSTRACTS

ARGON AS A CATALYST FOR METHYL MIGRATION IN $CH_3NO_2^+$

A. Cunje, V.I. Baranov, C.F. Rodriquez, A.C. Hopkinson and D.K. Bohme, York University, Department of Chemistry, 4700 Keele Street, Toronto, Ontario, Canada (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The barrier to the intramolecular 1,2-shift of a methyl group in the nitromethane cation in the gas phase is large. In solution such rearrangements are often catalyzed by the solvent and in principle a similar process can occur in the gas phase. Relative methyl cation affinities provide a guide as to what molecules might function as catalysts. In this study the inert gas argon was used as a catalyst. Optimizations and subsequent characterizations have been performed using Density Functional Theory (at B3LYP/6-311++G(d,p)) followed by single point calculations at QCISD(T)/6-311++G(2df,p). Experimental and theoretical results will be presented to show that argon does indeed function as an effective catalyst for methyl migration in $CH_3NO_2^+$.

THE EFFECTS OF REACTANT VIBRATION ON THE LIFETIMES AND FATE OF COLLISION INTERMEDIATES

S.L. Andreson, R.J. Green, H. Kim and J. Qian, (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Several multiphoton ionization schemes have been used to prepare molecular ions with variable excitation in selected vibrational modes. Reactions of these ions with other polyatomic molecules have been studied in a guided ion beam instrument that allows measurement of both integral cross sections and product recoil velocity distributions. In the reaction of phenol cations with ammonia, it is observed that both reactant vibrational mode and collision energy affect reaction cross sections. The reactions appear to go via a long-lived intermediate complex and this collision complex is stable enough to allow direct observation at low total energies. We are, thus, able to examine directly the effect of different modes of reactant excitation on complex lifetime and decomposition branching. For comparison, we also report a study of the analogous reactions starting in the opposite reactant charge state: ammonia cation(v)+phenol.

IN SITU MEASUREMENTS OF METHANE AND ACETYLENE CONCENTRATIONS IN A CVD REACTOR BY INFRARED SPECTROSCOPY

E. Canales, B.R. Weiner and G. Morell, Department of Chemistry, University of Puerto Rico-Rio Piedras, San Juan, PR 00931 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Measurements of the gas concentrations present during diamond growth can serve to test the various proposed mechanisms of diamond film deposition. In particular, the relative concentration of acetylene and methane is crucial to understand their role in the deposition process, as they are the most probable diamond precursors. We obtained in situ infrared spectra under conditions typical for diamond growth in a Hot Filament Chemical Vapor Deposition (HFCVD) system. We also took standard absorbance FTIR measurements of methane ($\nu_3(f_2)$ at 3020 cm^{-1} and $\nu_4(f_2)$ at 1306 cm^{-1} and of acetylene ($\nu_3(su+)$ at 3287 cm^{-1} and $\nu_4(612\ cm^{-1})+\nu_5$ at 1328 cm^{-1}) in the 5-50 torr range in order to calculate their absorption coefficients. These were then used in conjunction with the in situ infrared spectra to estimate the relative concentrations of acetylene and methane present close to the filament in our HFCVD system.

BROADBAND RINGDOWN SPECTRAL PHOTOGRAPHY

J.J. Scherer, J.B. Paul and A. O'Keefe, Los Gatos Research, 67 E. Evelyn Avenue, Suite #3, Mountain View, CA 94041 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

A new technique is presented which enables frequency resolved "cavity ringdown" absorption spectra to be obtained over a relatively large spectral region using a single pulse of broadband light. The ringdown spectral photography technique employs two key principles in order to record the time and frequency response of the optical cavity along orthogonal axes of a two-dimensional array detector. The approach enables the frequency dependent cavity decay times to be recorded as a two-dimensional image in a single-shot fashion. The image is subsequently analyzed to yield intracavity losses at a high spectral resolution over a large optical bandwidth. The ability to measure weak absorption with a sensitivity level comparable to that of conventional cavity ringdown spectroscopy is demonstrated. The microsecond timescale resolution of the technique is ideally suited for the real-time monitoring of ultra trace level chemical species.

CRLAS SPECTROSCOPY OF VINYL RADICAL: DYNAMICS IN THE EXCITED ELECTRONIC STATE

C.D. Pibel, Department of Chemistry, American University, Washington DC, A. McIlroy and C.A. Taatjes, Combustion Research Facility, Sandia National Laboratories, Livermore CA, and S. Alfred, K. Patrick and J.B. Halpern, Department of Chemistry, Howard University, Washington DC (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

High resolution (0.01 nm) vinyl radical (C_2H_3) $A^2A'' \leftarrow X^2A'$ absorption spectra have been measured using cavity ringdown spectroscopy. Line broadening is clearly observable, moving from the origin band to excitation of higher vibrational levels of the excited state. This definitive signature of unimolecular decay could not be seen in the only other published measurement of this spectrum by Hunziker et al. [*Can. J. Chem.* 61, 993 (1983)], taken at 1.6 nm resolution. We have been able to rotationally resolve the origin band and fit the envelope with a model for a c-type transition of an asymmetric top. For a best-fit, the model requires a 1 cm^{-1} Lorentzian linewidth, including laser and Doppler contributions, which corresponds to an excited state lifetime of about 50 ps. As the vibrational energy in the excited electronic state increases, the excited state lifetime decreases.

KINETICS AND BRANCHING RATIO MEASUREMENTS FOR THE METHYLPEROXY-NITRIC OXIDE REACTION

M.J. Elrod, K.W. Scholtens, B.M. Messer and C.D. Cappa, Department of Chemistry, Hope College, Holland, MI 49423 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The overall rate constant and an upper limit for the methyl nitrate product channel for the methylperoxy-nitric oxide reaction has been measured using the turbulent flow technique with high pressure chemical ionization mass spectrometry for the detection of reactants and products. The temperature dependence of the rate constant was investigated between 298 and 203 K at pressures of either 100 or 200 torr. Although the room temperature rate constant value agrees well with the current recommendation for atmospheric modeling, our values for the rate constant at the lowest temperatures accessed in this study are about 50% higher than the same recommendation. No methyl nitrate product was detected (using direct methyl nitrate detection methods for the first time) from this reaction, but an improved upper limit of 3% (at 298 K and 100 torr) for this branching channel was determined.

THE TEMPERATURE DEPENDENCE OF THE PRODUCT BRANCHING RATIO OF THE $CN+O_2$ REACTION

K.T. Rim and J.F. Hershberger, Department of Chemistry, North Dakota State University, Fargo, ND 58105 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The $CN+O_2$ reaction was studied over the temperature range 239-643 K using time-resolved infrared diode laser spectroscopy. The yield of the minor CO+NO product channel was quantified by direct measurement of the CO yield. The yield of NCO+O products was determined by measuring the N_2O yield upon addition of NO. Kinetic modeling simulations were performed to verify that the $NCO+O \rightarrow CO+NO$ secondary reaction did not significantly affect the measurements. We find that the CO+NO product channel is very minor at high temperatures, with a branching ratio of only $\phi=0.08$ at 643 K, but the yield of this channel increases at lower temperatures, with $\phi=0.28$ at 239 K.

MEASURED RATES OF DISSOCIATION OF PROPANE IN Ar, Ne, Kr AND Xe

J.P. Hessler and P.J. Ogren, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The rate of dissociation of propane diluted in Ar, Kr, Ne and Xe has been measured immediately behind incident shock fronts with the tunable-laser flash-absorption technique. The technique was improved by adding a second array detector to monitor pulse-to-pulse changes in the profile of the light beam. Measurements were performed at pressures near one atmosphere and over the temperature range 1300 to 3000 K. Our results in Kr agree with the earlier work of Al-Alami and Kiefer [*J. Phys. Chem.* 87, 499 (1983)].

The Master Equation and inverse Laplace transforms are used along with Monte Carlo simulations [*Int. J. Chem. Kinet.* 29, 803 (1997)] to extract the high-pressure and microcanonical rate coefficients and their bounds.

RATE CONSTANTS FOR THE REACTION OF CHLORINE WITH DEUTERATED METHANES

G.D. Boone, F. Agyin, F.-M. Tao and S.A. Hewitt, Department of Chemistry, California State University, Fullerton, CA 92834 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The rate constants for the reaction of Cl with deuterated methanes at 298 K and 1 atm were measured relative to the Cl reaction with CH_4 and CO using long path FTIR. The measured rate constants were found to be $6.5(\pm0.5)\times10^{-14}$, CH_3D; $4.2(\pm0.5)\times10^{-14}$, CH_2D_2; $1.9(\pm0.3)\times10^{-14}$, CHD_3; and $5.4(\pm0.5)\times10^{-15}$, CD_4(cm^3 $molecule^{-1}$ s^{-1} with uncertainties of 2σ). Ab initio calculations have also been made at the MP2 level with the 6-311G++(2d,2p) basis set. The kinetic isotope effect has been calculated using conventional transition state theory plus Wigner and Eckart semi-classical tunneling corrections. The theoretically calculated, Eckart corrected rate constants, relative to the $Cl+CH_4$ reaction rate constant of 1.0×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, were found to be 6.2×10^{-14}, CH_3D; 3.8×10^{-14}, CH_2D_2; 1.9×10^{-14}, CHD_3; and 4.4×10^{-15}, CD_4 (cm^3 $molecule^{-1}$ s^{-1}). The implications of this study for atmospheric chemistry and fundamental chemical reactivity are discussed.

VIBRATIONAL STATE CONTROL OF $H+N_2O$ BY STIMULATED RAMAN LASER EXCITATION

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The cross section for a bimolecular reaction can be dependent on reagent translational and internal energy. Experiments are underway to measure the reaction cross section for the reactions

$$H(E_t)+N_2O(n,l,m) = OH+N_2$$
$$= NH+NO$$

as a function of translational and vibrational energy. Calculations by Bradley and Schatz predict that reaction cross section is sensitive to translational energy while vibrational energy may play a crucial role in determining reaction pathway. Translationally excited H atoms are produced by laser photolysis of either HI or CH_3SH. Stimulated Raman excitation is used to prepare vibrationally excited and oriented $N_2O(n,l,m)$. The reaction will be monitored by sub-Doppler laser induced fluorescence of the OH and NH products.

LOW TEMPERATURE BEHAVIOR OF THE HYDROXYL RADICAL REACTING WITH NITROGEN DIOXIDE

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The temperature dependence of the termolecular rate coefficient of the hydroxyl radical with nitrogen dioxide has been studied between 76-242 K using a pulsed uniform supersonic flow reactor. This reaction pathway forms nitric acid that acts like a sink for NO_2. The radical OH concentration, prepared by pre-expansion cold cathode discharge in water vapor, was followed using $R_{21}(1)$ and $R_1(1)$ lines of the (1,0) band of the ($A\leftarrow X$) transition. Loss rates found as a function of NO_2 concentration and time yielded the association rates for various expansion temperatures. This study will be discussed in the context of current uncertainties in the nitric acid formation rates in the low temperature stratosphere.

REACTIVITY OF $C_5H_{11}N$ AMINES WITH O_2^+ AND NO^+ IN THE GAS PHASE

J.M. Van Doren, K.L. Cappuccio, M.F. Wszolek and S.K. Moses, Department of Chemistry, College of the Holy Cross, Worcester MA 01610 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The reactivity of all $C_5H_{11}N$ isomers with O_2^+ and NO^+ in the gas phase has been investigated at 300 K with a flowing afterglow. Rate coefficients and product branching fractions were determined and major secondary reactions identified. All isomers react efficiently with these ions. Reactions involving O_2^+ form nitrogen-containing product ions arising from loss of an alkyl group (beta to the nitrogen) from the neutral reactant. Reactions involving NO^+ form ionic products arising from charge transfer and hydride transfer. In addition, some fragmentation products are also observed. The chemical ionization mass spectra observed are similar to electron ionization mass spectra in many ways, suggesting that the former reactions are initiated by initial charge transfer.

SCALAR DISTRIBUTIONS AND ANGULAR CORRELATIONS OF NO TRAJECTORIES FROM PHOTODISSOCIATION OF TRIFLUORONITROSOMETHANE, 2-METHYL-2-NITROSOPROPANE, AND LARGE NITROSOALKANES

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Speed, energy and rotational population distributions, and angular correlations for the NO photofragment from the 585-650 nm photodissociation of selected nitrosoalkanes were measured using polarized REMPI with TOFMS detection. The NO speed distributions are consistent with dissociation on the T_1 surface except for CF_3NO, for which the S_0 surface dominates at dissociation wavelengths longer than 600 nm. A preference for $\mu \perp v_{NO}$ and $v \perp j_{NO}$ is observed for all compounds. Our results show that the fragmentation mechanism depends on the dissociation wavelength, NO rotational state, and the rigidity of molecular skeleton. For CF_3NO the dynamics is observed to depend on the spin-orbit state of the NO product.

PHOTODISSOCIATION OF METHYL IODIDE AT 193.3 nm: THE H-ATOM CHANNEL

G. Amaral, K. Xu and J. Zhang, Department of Chemistry and Air Pollution Research Center, University of California, Riverside, CA 92521 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

While the CH_3+I channel in the ultraviolet photodissociation of CH_3I has been extensively studied, the H atom channel receives little attention. In this work, the H(D)-atom channel in the photodissociation of jet-cooled CH_3I and CD_2HI at 193.3 nm has been investigated by using the high-n Rydberg-atom time-of-flight technique. CM kinetic energy distributions have been obtained for both molecules. The upper limits of the bond energy are $D_0(CH_2I\text{-}H) = D_0(CD_2I\text{-}H) = 101(\pm 1)$ kcal/mol and $D_0(CDHI\text{-}D) = 102.5(\pm 1)$ kcal/mol. In CH_3I, 80% of the available energy is channeled in product translation and 17% in vibration. C-I stretch and out-of-plane umbrella modes of the CH_2I radical have been observed. The energy partitioning and product vibrational excitation are similar in CD_2HI. Angular distribution measurements reveal different spatial distributions for the H-atom channels from CH_3I and CHD_2I and the D-atom channel from CHD_2I. Photodissociation mechanisms are discussed.

ULTRAVIOLET PHOTODISSOCIATION DYNAMICS OF ETHANOL

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193.3 nm photodissociation of jet-cooled C_2H_5OH and C_2H_5OD has been studied by using high-n Rydberg-atom time-of-flight technique. Isotope labeling study shows that H-atom fragment is produced preferentially from O-H bond fission. Center-of-mass (CM) kinetic energy distribution of the H(D) atom and ethoxy radical photofragments has been obtained. Average CM translational energy is very large, with $f_T=0.83$ for $H+C_2H_5O$ and $f_T=0.79$ for $D+C_2H_5O$. An upper limit of the bond dissociation energy is $D_0[C_2H_5O\text{-}H(D)]=103.3(\pm0.5)(105.9\pm0.5)$ kcal/mol. The CM translational energy distribution of the C_2H_5O+H products reveals C-C-O bending and C-O stretching excitation in the C_2H_5O radical. The anisotropic parameter of the photofragments is -0.9, indicating a perpendicular electronic transition at 193.3 nm. The obtained dynamic information implies that the C_2H_5O+H channel in 193.3 nm photodissociation of ethanol occurs via a prompt dissociation process and on a repulsive excited-state potential energy surface.

ION IMAGING MEASUREMENTS OF THE STEREODYNAMICS OF 2-CHLORO-2-NITROSOPROPANE PHOTODISSOCIATION

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The ion imaging technique was applied to study angular correlations in the trajectory of the NO product from photodissociation of 2-chloro-2-nitrosopropane. The results confirm earlier TOF studies: the NO velocity vector, v, is perpendicular to its angular momentum, j, ($\beta_0^0(22)=-0.206$) and there is no significant correlation between v and the transition dipole moment, μ, of the parent molecule ($\beta_0^2(20)=-0.020$). The recoil velocity distribution shows two features - a broad slow and a narrow fast components with average values of approximately 250 and 900 m/s respectively. These components are assigned to dissociation from the S_0 and T_1 technique, allowing direct modeling of the angular correlation in ion images, which has significant advantages over the less general Abel transform method.

POTENTIAL ENERGY SURFACES FOR THE PHOTODISSOCIATION OF SMALL MOLECULES

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The ab initio computation of potential energy surfaces for photodissociation processes can be extremely demanding due to the large electron correlation and basis set requirements for accurate results, particularly when multiple electronic states are being treated. Potential energy surfaces to describe the photodissociation of HOBr and OClO have been computed at the multireference CI level of theory. In the case of HOBr, a total of five electronic states have been treated for the OH+Br channel. For OClO, preliminary calculations have centered on the excited A-state leading to ClO+O. General features of these surfaces will be presented, including preliminary calculations of spin-orbit coupling effects. Methods of utilizing basis set convergence properties to yield more accurate surfaces, as well as various analytical fitting strategies will be discussed.

PHOTODISSOCIATION DYNAMICS OF HONO AT 193.3 nm

J. Zhang, G. Amaral and K. Xu, Department of Chemistry and Air Pollution Research Center, University of California, Riverside, CA 92521 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Nitrous acid (HONO) is an important atmospheric species. Photodissociation of HONO at 193.3 nm has been examined by using high-n Rydberg hydrogen-atom time-of-flight technique. Center-of-mass (CM) translational energy distribution of the products has revealed, for the first time, that the NO_2 fragments are produced in several electronic states: ground state X^2A_1 and excited states A^2B_2 and B^2B_1 or C^2A_2. The CM translational energy distribution also shows that NO_2 vibration is highly excited in each of these electronic states. In particular, a long bending progression of NO_2 in A^2B_2 state has been observed. Angular distribution measurement of the H-atom products by using the polarized photolysis radiation demonstrates a nearly isotropic spatial distribution for all the product channels. Branching ratios of the different NO_2 electronic states have been obtained. Photodissociation mechanism of HONO at 193.3 nm is discussed.

EXPLORING INTRAMOLECULAR DYNAMICS IN THE FREQUENCY DOMAIN AND TIME DOMAIN BY PHOTODISSOCIATION OF VIBRATIONALLY EXCITED MOLECULES

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Photodissociation of a vibrationally excited molecule allows one to explore both ground and electronically excited state processes. Because the photolysis is sensitive to the vibrational state from which the dissociation occurs, it is possible to use vibrational state selective photodissociation to probe intramolecular dynamics spectroscopically (frequency domain measurements) or temporally (time domain measurements). An example of a frequency domain measurement is the vibrational spectroscopy in the region of three quanta of N-H stretch in isocyanic acid (HNCO) molecules cooled in a molecular beam. An example of a time domain measurement is the direct observation of energy flow in nitric acid (HNO_3) in which a 100 fs laser pulse prepares an O-H stretching vibration and another pulse dissociates the molecules following energy redistribution. Both approaches provide a means of controlling reactions, including nonadiabatic processes.

EXTENDED SPECTRAL CROSS-CORRELATION APPLIED TO THE STATE-RESOLVED PHOTOFRAGMENTATION DYNAMICS OF DEUTERATED AMMONIA SPECIES

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The technique of spectral cross-correlation is extended to study the photodissociation dynamics of partially deuterated ammonia species, probed by time-resolved Fourier transform infrared emission spectroscopy. This pattern recognition technique enables the identification and separation of spectral features that are characteristic of the dissociation products from each of the four parent molecules (NH_3, NH_2D, ND_2H and ND_3) present in equilibrated mixtures of varying composition. Nascent NH_2 and ND_2 product distributions from the dissociation of NH_2D and ND_2H, respectively, in their first electronically excited state, are vibrationally more excited than those from the dissociation of NH_3 and ND_3, and a larger proportion of energy is also partitioned into rotation about the minor b/c-axes of rotation. These observed trends can be attributed to the vibrational modes excited at the photolysis wavelength of 193 nm and thus the differing dissociating geometries sampled by the parent molecules. In addition to the nascent

distributions extracted for each parent dissociation, the estimated branching ratios for N-H vs N-D bond cleavage afford new insights into the photofragmentation dynamics of ammonia.

FRAGMENT RECOIL ANISOTROPY IN NO_2 PHOTODECOMPOSITION

A. Demyanenko, V. Dribinski and H. Reisler, University of Southern California Chemistry Department, Los Angeles, CA 90089 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The photodecomposition of NO_2 at 339, 355 and 373 nm is studied using photofragment velocity map imaging in conjunction with REMPI detection of the nascent products NO(v,J) and $O(^3P_J=0,1,2)$. Probing the angular and energy distributions of each state-selected fragment provides detailed insight into the dissociation dynamics at long range. The rovibrational distributions of the NO co-fragment are obtained from the translational energy distribution of $O(^3P_J)$. A strong dependence of the recoil anisotropy parameter on internal energy of the NO photofragment and the recoil energy is revealed. From images of NO(v,J) states it is concluded that for pairs with the same recoil energy, higher NO rotational energy is associated with lower value of the anisotropy parameter. The detailed dependence of the parameter on vibrational and rotational energy of NO and the oxygen atom spin-orbit state will be discussed.

FEMTOSECOND MULTIPHOTON IONIZATION OF PHENOL

P.M. Weber and C.P. Schick, Department of Chemistry, Brown University, Providence, RI 02912 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Electronic relaxation processes in phenol are studied using a molecular beam apparatus with a time-of-flight photoelectron spectrometer. Upconverted third and fourth harmonic femtosecond laser pulses from a regenerative amplifier system are used to excite phenol to the first or second excited singlet state, S_1 or S_2. By ionizing via the S_2 state resonance, we observe a competition between internal conversion from S_2 to S_1 and direct ionization from S_2. Analysis of the photoelectron spectra taken at different resonant wavelengths suggests that the potential of the S_2 state is displaced from the S_0 state along the 6a normal mode coordinate. We also observe evidence for above-threshold multiphoton ionization of phenol when ionizing via the S_1 state resonance. The resulting photoelectron spectra show a greater propensity for an electronically excited ion state than for the ground ion state, as well as an unusually long vibrational progression spanning more than 12,000 wavenumbers.

INTRAMOLECULAR AND UNIMOLECULAR DYNAMICS OF REACTIVE INTERMEDIATES WITH SHALLOW POTENTIAL ENERGY WELLS

W.L. Hase, Department of Chemistry, Wayne State University, Detroit, MI 48202 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Experimental and theoretical/computational studies have suggested that IVR may not compete with decomposition for unimolecular reactions with shallow potential energy wells. The lifetime for the intermediate is much shorter than the time for IVR and the result is non-RRKM kinetics. This type of behavior may be important for numerous reactions and, from classical chemical dynamics simulations, has been implicated for S_{N2} ion-molecule complexes and for the trimethylene intermediate in cyclopropane isomerization. For the $Cl^- + CH_3Cl$ S_{N2} reaction, a direct reaction is observed without ion-dipole complex formation if the reactant C-Cl stretch is excited. The complex, when formed, exhibits mode specific kinetics. Cyclopropane ring opening, to form the trimethylene biradical, may occur via three different transition states. When the biradical undergoes ring closer, to form a geometric isomer, it retains a memory of how it was formed.

STATE RESOLVED STUDIES OF DISSOCIATIVE UNIMOLECULAR DYNAMICS

F. Temps, Institut fur Physikalische Chemie, Olshausenstr. 40, 24098 Kiel, Germany (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

We have investigated the intramolecular kinetics and the dissociative unimolecular dynamics of a series of chemically interesting free radicals, namely CH_3O and $CH_2DO(X^2E)$ and HCO, and $DCO(X^2A')$. Experiments were performed at a fully quantum state resolved level of detail using the methods of dispersed fluorescence spectroscopy and stimulated emission pumping. Detailed information was obtained for the above systems pertaining to their distinctive vibrational structures and the ensuing vibrational dynamics (in particular regarding the Jahn-Teller effect in CH_3O and CH_2DO and anharmonic coupling effects in DCO), the state densities, effects of rotational excitation on the state resolved decay constants, and implications of the state resolved results for thermal reactions. Selected aspects will be highlighted and discussed.

ORDER OUT OF CHAOS: LOCAL BENDS ABOVE THE ENERGY OF THE ACETYLENE-VINYLIDENE ISOMERIZATION BARRIER

R.W. Field and M.P. Jacobson, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Acetylene dispersed fluorescence spectra are observed up to 5000 cm^{-1} above the barrier to acetylene-vinylidene isomerization. Pattern recognition is used to disentangle overlapping spectral features belonging to different polyads. Separating the spectrum into polyads, free of assumptions about the number or nature of polyad patterns, implies the exact Hamiltonian can be block diagonalized into effective Hamiltonians. The form of the polyad H^{eff} is influenced by the isomerization path. A regular, large amplitude, local bender motion emerges in the pure-bending polyads at high E_{vib}. This local motion follows the isomerization path up to a bend angle close to the isomerization transition state. Predicted and observed spectral patterns agree at E_{vib} well above this barrier. The spectrum and dynamics (depicted by survival and transfer probabilities and number operator expectation values) are simpler at E_{vib}=15,000 cm^{-1} than at 10,000 cm^{-1}.

AB INITIO DYNAMICS OF THE VINYLIDENE-ACETYLENE ISOMERIZATION VIA VINYLIDENE RADICAL ANION ELECTRON DETACHMENT

R.L. Hayes, E. Fattal, N. Govind and E.A. Carter, Department of Chemistry and Biochemistry, Box 951569, University of California at Los Angeles, Los Angeles, CA 90095 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

We present an ab initio molecular dynamics (AIMD) simulation of the negative ion photodetachment-induced isomerization of vinylidene to acetylene. Ervin et al. Measured the vibrational structure and isomerization dynamics of vinylidene by measuring the photoelectron spectrum of the geometrically similar vinylidene anion. We model this system with AIMD at the CASSCF level. After equilibrating the vinylidene anion at finite temperature, an electron is removed to form singlet vinylidene. Twenty distinct vinylidene trajectories are followed for 0.44 ps or until they isomerize. Trajectories generated from the isomerization transition state are also calculated for comparison. Using filter diagonalization, dynamic anharmonic vibrational frequencies are extracted, allowing direct comparison of molecular motion with experimental spectra.

THE ROLE OF ROTATIONAL ENERGY ON THE UNIMOLECULAR DISSOCIATION OF KETENE

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The unimolecular dissociation of ketene as one of the simplest elementary dissociation reactions proceeding via two different channels (i.e. the singlet and triplet methylene channels) has been investigated by ps pump probe experiments which provide direct time resolved information of the unimolecular decay. Beyond photodissociation of non-rotating "cold" molecules the impact of rotation on unimolecular dissociation has recently attracted considerable attention. In our contribution we compare direct time resolved measurements of the singlet methylene channel in a supersonic jet and in a thermal sample with predictions from a statistical adiabatic channel model for different rotational temperatures. This approach enables us to elucidate the role of angular momentum, its projection K on the molecular axis, as well as the energy partition between rotational and vibrational degrees of freedom in the unimolecular dissociation of ketene.

THE FRAGMENTATION SURFACE OF TRIPLET KETENE

W.D. Allen, R.A. King and H.F. Schaefer III, Center for Computational Quantum Chemistry, Department of Chemistry, University of Georgia, Athens, GA 30602 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

A rigorous mapping and analytic parameterization has been performed of the TZ(2d1f,2p) CCSD intrinsic reaction path connecting triplet ketene to $CH_2(^3B_1)+CO(^1\Sigma^+)$ through its in-plane bent transition state. Functional forms have also been developed for all quadratic force field elements along this path, allowing analytic computation of curvature couplings and all other quantities in the corresponding reaction path Hamiltonian. Final potential energy functions along the fragmentation path have been determined with the aid of [(C,O)/H] atomic-orbital basis sets as large as [6s5p4d3f2g1h/5s4p3d2f1g] and electron correlation treatments as extensive as coupled-cluster methods through triple and quadruple excitations [CCSDT, CCSD(T), and CCSD(TQ)]. The final theoretical curve is highly anharmonic in the transition state region, displaying a classical barrier of 988 cm^{-1}, a critical C-C distance of 2.262 A, and a barrier frequency of 317i cm^{-1}. Effective barrier frequencies in the 100i cm^{-1} range which result from RRKM modeling with tunneling corrections of the observed steplike structure in the triplet ketene dissociation rate constant are thus shown to be physically untenable. Various implications of such ab initio predictions on unraveling the intricacies of the fragmentation dynamics in this paradigmatic system are discussed.

FEMTOSECOND PHOTOIONIZATION STUDIES OF ACETYL UNIMOLECULAR DECOMPOSITION

A.P. Baronavski and J.C. Owrutsky, Chemistry Division, Naval Research Laboratory, Washington, DC 20375 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Femtosecond photoionization spectroscopy has been used to measure unimolecular decay rates for acetyl produced by photodissociation of acetic acid and acetyl cyanide near 200 nm. Acetyl precursors with simple (diatomic) accompanying fragments and well characterized product energy distributions, such as for these precursors, permit quantitative investigation of the dissociation dynamics. Agreement between the observed lifetimes and RRKM lifetimes at the average internal energy is poor, especially for acetic acid. But the agreement is greatly improved when the energy distribution (the shape of the distribution) of the acetyl is properly taken into account. In addition, ab initio calculations have been used to determine that the acetyl cyanide absorption band at 195 nm is due to a π-π^* transition.

DETERMINING CRITICAL ENERGIES FOR UNIMOLECULAR REACTIONS: THE DECOMPOSITIONS OF C_2H_4F RADICALS AND CYCLOBUTENE

D.C. Tardy, Department of Chemistry, University of Iowa, Iowa City, IA 52242, R.P. Thorn Jr, W.A. Payne Jr and L.J. Stief, Laboratory for Extraterrestrial Physics, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, and F.L. Nesbitt, Department of Natural Sciences, Coppin State College, Baltimore, MD 21216 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Highly vibrationally excited radicals or molecules have been formed by the addition of F atoms to ethylene or the combination of vinyl radicals These chemically activated (CA) species can undergo competitive collisional stabilization or unimolecular reaction. RRKM calculations have been performed for the decomposition of CA C_2H_4F radicals (open shell) as a function of temperature and pressure for various energy transfer models. Comparison of these calculations with recent experimental results indicate that the critical energy for $F+C_2H_4$ is about 5 kcal/mole higher than that for $H+C_2H_3F$. The results of RRKM calculations for competitive processes in CA 1,3-butadiene (closed shell) indicate that the CA 1,3-butadiene has sufficient energy to isomerize to cyclobutene and then decompose to C_2H_2 and C_2H_4. The importance of the energy transfer model on these systems will be discussed.

VIBRATIONAL LEVELS OF THE TRANSITION STATE AND RATE OF DISSOCIATION OF TRIPLET ACETALDEHYDE

I.-C. Chen, Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, ROC 300 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Photodissociation dynamics and relaxation mechanism of acetaldehyde in electronic excited states are studied. Rates of appearance of DCO from dissociation of acetaldehyde are measured. The stepwise increases in plots of both rate of appearance of formyl radicals and rate of decay of excited acetaldehyde vs. excitation energy for both isotopic variants of acetaldehyde are observed. These sharp increases correspond to vibrational levels of transition state in the triplet surface. Frequencies of torsional and C-C-O bending modes are determined to be 73(±10) cm^{-1} and 200(±10) cm^{-1} for the transition state of CD_3CDO and the torsional frequency 80(±10) cm^{-1} for CH_3CHO. From these fits the dissociation threshold for formation of radical fragments is determined to be 31845 cm^{-1} for CD_3CDO and 31650 cm^{-1} for CH_3CHO.

QUANTUM DYNAMICS OF UNIMOLECULAR REACTIONS

S.K. Gray and C.-Y. Yang, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Quantum mechanical approaches for obtaining unimolecular resonance properties will be briefly outlined. The results of full dimensional, numerical studies of the unimolecular dissociation reactions

$HCO \rightarrow H+CO$
$HOCl \rightarrow Cl+OH$ and
$H_2O \rightarrow H+OH$

will then be discussed. All the calculations employ accurate, ab initio based potential energy surfaces for the corresponding ground electronic states. In the case of HCO, the influence of total angular momentum on resonance properties is noted. In the cases of HOCl and H_2O, the focus is on the behavior of low-lying resonances not too far removed from the reaction thresholds. Some H_2O resonances are found with clear local mode character.

INTRAMOLECULAR ENERGY TRANSFER AND UNIMOLECULAR DISSOCIATION DYNAMICS OF ROTATIONALLY STATE-SELECTED HOCl

T.R. Rizzo, J. Rebstein, A. Callegari, R. Jost and J.S. Muenter, Laboratoire de Chime Physique Moleculaire, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland
(Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Infrared-optical double resonance excitation of OH stretch overtone transitions in HOCl prepares reactant molecules in single rovibrational states above the threshold for dissociation to OH + Cl. Frequency domain spectra of these quasibound levels reveal the nature of the doorway states that couple most strongly to the excited OH stretch vibration and hence the path of energy flow out of this mode. Spectroscopic detection of the dissociation products in time reveals unimolecular dissociation rates that fluctuate as much as two-orders magnitude between adjacent states. We use the combination of frequency- and time-resolved results in an attempt to provide a detailed picture of the chemical bond breaking dynamics.

ION IMAGING STUDIES: STATISTICS, DYNAMICS AND MULTIPLE PATHWAYS IN UNIMOLECULAR COMPOSITIONS

H. Reisler, University of Southern California Chemistry Department, Los Angeles, CA 90089
(Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Unimolecular reactions are often induced by photoexcitation to bright electronic states. The ensuing dynamics involves either vibrational predissociation on the bright state, or radiationless transitions to lower states that are coupled to dissociation continua. The competition among these processes can lead to the appearance of several distinct channels whose branching ratios depend sensitively on the characteristics of the potential energy surfaces and crossing seams. Photofragment velocity map imaging has been used to determine barrier heights and time scales in the photodecomposition of HNCO to three competing channels, thereby revealing energy flow mechanisms, and in particular the coexistence of nonadiabatic pathways in competition with fast, direct dissociation channels. The influence of long-range forces on the barrierless unimolecular decomposition of HNCO to H + NCO and NO_2 to NO and O will also be discussed.

NO_2 ® NO + O: ROTATIONAL DEPENDENCE OF THE UNIMOLECULAR REACTION RATE

I. Bezel and C. Wittig, Department of Chemistry, University of Southern California, Los Angeles, CA 90089
(Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The dependence of the rate of photoinitiated NO_2 unimolecular decomposition on parent rotation has been measured just above D_0 by using IR-UV double resonance. Rotational selectivity was achieved by using narrow linewidth IR radiation to prepare a particular rotational state [$N = 1,3,..15$, $K_a = 0$; $E_{rot} = BN(N+1)$] of the (1,0,1) combination band. The picosecond pump-probe technique was used to photodissociate these tagged molecules and to monitor the rate of appearance of the NO product. Data were recorded with two UV photon energies whose values are $D_0 + 18$ cm^{-1} and $D_0 + 83$ cm^{-1}. The measured rates do not exhibit any noticeable dependence on N. This reflects significant rovibrational interaction. The spin-orbit mechanism which was thought to be the main source of rovibronic interaction for small values of N is not likely to give such a result. A model is proposed to describe the influence of rotation on the dissociation rate. The data are consistent with the participation of Coriolis coupling of different K_a. The average reduced matrix element is estimated to be about 0.3 cm^{-1}.

ARE SEMICLASSICAL METHODS ACCURATE FOR ELECTRONICALLY NONADIABATIC TRANSITIONS BETWEEN WEAKLY COUPLED POTENTIAL ENERGY SURFACES

Y.L. Volobuev, M.D. Hack and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *J. Phys. Chem.* A).

We have performed a systematic series of semiclassical and quantum mechanical calculations of collisions of Br* (electronically excited Br) with H_2 in order to test four semiclassical methods against accurate quantum mechanical scattering calculations for the quenching probability and the electronically nonadiabatic reaction probability. The results are analyzed using four different methods of assigning final quantum numbers based on the final values of the semiclassical and classical trajectory variables, namely energy-non-conserving histogram analysis, energy-conserving histogram analysis, energy-non-conserving linear smooth sampling, and energy-conserving linear smooth sampling. We examine the use of both forward and reverse state-to-state probabilities to predict the quenching and reaction probabilities. The reaction and quenching probabilities are compared to the results of accurate quantum mechanical calculations, and the mean unsigned error is calculated for each combination of a semiclassical method and a final analysis algorithm. Our results indicate that Tully's fewest switches (TFS) trajectory-surface-hopping method and the Ehrenfest self-consistent-potential method show the best agreement with the accurate results, although none of the methods provides satisfactory agreement in the cases where the reaction or quenching probability is small. The TFS method is the only one that can be used to calculate the reaction probabilities for this system directly in the forward direction, and it is judged to be the best method overall for weakly coupled potential energy surfaces.

MECHANISM OF THE NITROUS ACID FORMATION FROM THE HYDROLYSIS OF NITROGEN DIOXIDE

F.-M. Tao and A. Chou, Department of Chemistry, California State University, Fullerton, CA 92834 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

The reaction mechanisms for the production of nitrous acid (HONO) from the hydrolysis of nitrogen dioxide under atmospheric conditions are studied by density functional theory and ab initio methods. The molecular structures and energies of the NO_2-H_2O systems along several reaction pathways are calculated using the B3LYP method with the 6-31G* and 6-311+G(2d,p) basis sets. The reaction pathways represent homogeneous hydrolysis of the NO_2 monomer and dimer with varying number of water molecules. The introduction of excess water molecules greatly stabilizes the transition state and reduces the activation energy in the monomer reactions. The reactions of the dimer are always favored over the monomer reactions. The formation of nitrous acid appears to involve multiple competing pathways with relative contributions sensitively dependent on system parameters such as humidity, pressure and temperature.

INTRAMOLECULAR VIBRATIONAL DYNAMICS OF HIGHLY EXCITED METHANOL STUDIED BY ROTATIONALLY RESOLVED OVERTONE SPECTROSCOPY

O.V. Boyarkin, D.S. Perry and T.R. Rizzo, Laboratoire de Chime Physique Moleculaire, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Double resonance excitation, together with cooling in a supersonic free jet, permits the measurement of overtone spectra of rotationally state-selected molecules. Application of this frequency domain approach to study the dynamics of the highly excited OH stretch vibration in methanol up to v=8 reveals three times scales of IVR. The shortest (subpicosecond) time scale corresponds to large spectral splittings caused by specific strong couplings. The secondary time scale (typically 1-10 ps) corresponds to smaller spectral splittings arising from weaker low-order couplings to a restricted number of states. The third and longest observable time scale

corresponds to extensive vibrational energy redistribution to a significant number of states. The rate of this third process increases nearly exponentially with vibrational energy, finally converging with the two faster scales at about 25,000 cm^{-1} of vibrational energy.

EFFECTS OF DONOR POLARITY ON THE MAGNITUDE AND PARTITIONING OF ENERGY TRANSFER FROM HIGHLY VIBRATIONALLY EXCITED MOLECULES TO WATER

M.S. Elioff, M. Fraelich and A.S. Mullin, Department of Chemistry, Boston University, Boston, MA 02215 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

We have performed experiments to investigate the influence of long-range attractive forces on collisional energy loss from highly vibrationally excited molecules. State-resolved studies of energy transfer from highly vibrationally excited pyridine (μ=2.2 D) to water (μ=1.8 D) have been performed in low pressure at 300 K using high resolution transient absorption spectroscopy at about 2.7 μm from a tunable F-center laser. Vibrationally excited, electronic ground state pyridine with E_{vib}=37900 cm^{-1} was prepared by absorption of pulsed ultraviolet light (266 nm) to the S_1 state followed by rapid radiationless decay to the S_0 state. Collisional quenching of vibrationally excited pyridine by water which results in rotational and translational excitation of H_2O (000) was investigated by monitoring the appearance of individual rotational states of H_2O (000) using the highly allowed asymmetric stretching transition (000$\rightarrow$001). Transient absorption population measurements reveal information about the nascent distribution of rotational energy of water. Doppler-broadened lineshapes provide data on the velocity distributions of recoiling water molecules. Bimolecular energy transfer rate constants provide information about the importance of the V$\rightarrow$R/T pathway. The results of these experiments were compared to energy transfer studies performed in this laboratory between pyrazine (μ=0 D) and water. This comparison permits insight into the effects of donor molecule polarity on the mechanism of energy transfer.

MOLECULAR DYNAMICS STUDIES OF INTRAMOLECULAR VIBRATIONAL ENERGY FLOW IN OVERTONE-EXCITED HYPOCHLOROUS ACID

J. Tian, K.N. Houk and R.D. Levine, Department of Chemistry and Biochemistry, University of California at Los Angeles, CA 90095 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Computational studies of intramolecular vibrational energy redistribution (IVR) in HOCl excited to above its first dissociation limit (O-Cl bond breaking) were carried out with density functional theory generated potential energy surface. As in recent experimental studies, the initial state was chosen such that the vibrational excitation was localized in the O-H stretch motion. The time evolution was determined by classical mechanics; for each nuclear configuration reached by the trajectory, the potential energy and its gradients were directly computed using the density functional theory at the B3LYP/6-31G* level. The trajectories were integrated for times up to 1 ps. A direct view of the intramolecular vibrational energy flow of HOCl initiated on its $7\nu_{OH}$ and $10\nu_{OH}$ vibrational excited state is presented. It is found that there is hardly any direct energy transfer between the O-H stretch and the O-Cl stretch. Rather, the energy needed for dissociation flows first from the O-H stretch to the H-O-Cl bend motion. The stretch to bend coupling is facilitated by (anharmonic) resonance as demonstrated by initiating trajectories with 10 quanta of O-H stretch.

FAST IVR: HOW GOOD AN ASSUMPTION IS IT IN LARGE MOLECULES?
M. Gruebele, School of Chemical Sciences and Beckman Institute, University of Illinois, Urbana, IL 61801 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

A series of models ranging from simple local random matrices to ab initio based potential surfaces, together with experimental data collected by our and other groups, are examined to determine how rapidly IVR goes to a completion in organic molecules. We find that dephasing takes place on a manifold embedded in state space which is considerably lower-dimensional than 3N-6 for large nonlinear molecules. An expression for the dimensionality of this manifold in terms of molecular parameters is given using analytical and computational results. As a result, IVR proceeds via "diffusive" power-law dynamics once the perturbatively treatable initial "Golden-Rule" decay period has elapsed, although the exponents are non-classical due to quantum-interference effects. IVR is therefore very sluggish after an initially fast period. While the early limited energy redistribution will generally be sufficient for the "fast randomization hypothesis" to be applicable to many measurements, more sophisticated coherence-manipulation experiments could show IVR to be a practicably reversible process.

G2 WITH PROPER DISSOCIATION, IMPROVED ACCURACY AND LESS COST
P.L. Fast, M.L. Sanchez, J.C. Corchado and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *J. Chem. Phys.*).

The empirical Gaussian-2 method (G2) of Pople et al. has been an enormously successful tool for computational thermochemistry, as reviewed elsewhere. There have been many attempts to devise modified G2 methods, typically to decrease the computational cost without a great loss in accuracy by substituting less expensive alternatives for some of the steps, although there have also been successful attempts to improve the accuracy by making changes in the method. In this paper we present two simple modifications of G2 that use a subset of the calculations used in the G2 method, but improve its accuracy for atoms in the Li-Ne period by almost a factor of two with a 10% reduction in cost.

INFINITE BASIS LIMITS IN ELECTRONIC STRUCTURE THEORY
P.L. Fast, M.L. Sanchez and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in *J. Chem. Phys.*).

We have developed a database of 29 molecules for which we have estimated the complete-one-electron-basis-set limit of the zero-point-exclusive atomization energy for five levels of electronic structure theory: Hartree-Fock theory, Moller-Plesset second- and fourth-order perturbation theory, coupled cluster theory based on single and double excitations (CCSD), and CCSD plus a quasiperturbative treatment of triple excitation (CCSD(T)), all at a single set of standard geometries. The estimates are believed to be correct to within a few tenths of a kcal/mol or better. This databse is then used to obtain optimized power-law exponents for extrapolating to the basis-set-limit from correlation-consistent polarized valence double and triple zeta (cc-pVDZ and cc-pVTZ) basis sets. This allows one to get thermochemical accuracy comparable to quadruple or quintuple zeta (cc-pVQZ or cc-pV5Z) basis sets with a cost very comparable to triple zeta, which is one order of magnitude less expensive than quadruple zeta and two orders of magnitude less expensive than quintuple zeta.

AB INITIO ENERGETICS FOR ETHANE AND DIMETHYL ETHER COMBUSTION

N.T. Quach, W.F. Schneider and E.A. Carter, Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Dimethyl ether has the potential to be a clean-burning diesel fuel. While ethane combustion energetics have been well characterized previously, DME combustion is not well understood. We present comparisons of the predictions of various explicit correlation methods (e.g., CASSCF and GVB-MP2) versus density functional theory (DFT) with the B3LYP semiempirical exchange-correlation functional and versus experiment, for the reaction energetics of both ethyl radical and methoxymethyl radical with O_2. Preliminary findings suggest that B3LYP-DFT yields much more accurate energetics for ethane combustion. We will present results for dimethyl ether combustion, in order to determine if B3LYP-DFT is robust enough to also reproduce the known thermochemistry in this system.

PHOTOIONIZATION STUDIES OF HO_2 AND H_2O_2: ENTHALPY OF FORMATION OF HYDROPEROXYL RADICAL

B. Ruscic and M. Litorja, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 (Presented at the *217th National Meeting of the American Chemical Society*, Held in Anaheim CA, March 1999).

Hydroperoxyl radical was generated in situ from H_2O_2 by hydrogen abstraction with F atoms. The adiabatic ionization energy of HO_2 is 11.352(±0.007) eV. The threshold behavior of HO_2^+ fragment from H_2O_2 can be analyzed relative to the OH^+ fragment in terms of appropriate model functions and leads to a 0 K fragment appearance energy of HO_2^+ from H_2O_2 of 15.112(±0.035) eV, and hence D_0(H-OOH) = 86.7(±0.8) kcal/mol (87.9±0.8 kcal/mol at 298 K), implying a 0 K enthalpy of formation of HO_2 of 4.0(±0.8) kcal/mol (3.3±0.8 kcal/mol at 298 K). The resulting proton affinity of O_2 is 100.6(±0.8) kcal/mol, while the 298 K enthalpy of deprotonation of hydrogen peroxide is 376.4(±0.8) kcal/mol. These experimental results are compared to ab initio calculations at the G2 and G3 levels of theory.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

JANUARY 7-9, 1999

SPECTROSCOPY OF RADICALS AND IONS: HIGH RESOLUTION SPECTROSCOPY GROUP MEETING OF THE ROYAL SOCIETY OF CHEMISTRY
Southampton, UK.

Information: S. Riaz, The Royal Society of Chemistry, Burlington House, London, W1V 0BN, UK, e-mail: riazs@rsc.org

JANUARY 10-14, 1999

EUROPEAN WINTER CONFERENCE ON PLASMA SPECTROCHEMISTRY
Pau, France.

Information: Congress Rive Droite, 28 rue Baudrimont, 33100 Bordeaux, France, 33(556) 32 82 29, Fax 33(556) 32 79 53.

JANUARY 11-14, 1999

37th AIAA AEROSPACE SCIENCES MEETING AND EXHIBIT
Reno NV.

Information: R.L. Cook, Mississippi State University, 320 Etheredge Engineering Building, P.O. Drawer MM, Mississippi State, MS 39762, (601) 325 2105, Fax (601) 325 8465, e-mail: cook@dial.msstate.edu

JANUARY 17-22, 1999

GORDON RESEARCH CONFERENCE ON THE CHEMISTRY OF HYDROCARBON RESOURCES
Ventura CA.

Topics Include:
- Hydrocarbon Resources in the 21st Century
- Advances in Compositional and Instrumental Approaches to Hydrocarbon Chemistry
- Computational Approaches to Hydrocarbon Reaction Chemistry
- Frontiers of Catalysis in Hydrocarbon Reactions
- High-Temperature Hydrocarbon Chemistry
- Advances in Carbon Materials: Nano-Structures and Catalysts
- Membrane Reactors
- Advances in Methane Conversion Chemistry

Information: J.H. Shinn, Chevron Research and Technology, e-mail: shis@chevron.com or http://www.grc.uri.edu

JANUARY 21-26, 1999

ANNUAL MEETING OF THE AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE
Anaheim CA.

Information: E. Cooper, AAAS, (202) 326-6431, Fax (212) 789-0455, e-mail: ecooper@aaas.org, http://www.aaas.org/meetings/scope

JANUARY 22-24, 1999

INTERNATIONAL SYMPOSIUM ON CLEAN COAL INITIATIVES
New Delhi, India.

Information: T.N. Singh, Chairman, Organizing Committee, CCI 99 and Director Central Mining Research Institute, Barwa Road, Dhanbad 826 001, Bihar, India, 91(326) 202326/ 203043, EPBX 91(326) 203070/203090, Fax 91(326) 202429/205028,
e-mail: director@cscmri.ren.nic.in; root@cscmri.ren.nic.in

JANUARY 23-29, 1999

LASE '99: HIGH POWER LASERS AND APPLICATIONS
San Jose CA.

One of the International Symposia at Photonics West.
Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JANUARY 24-27, 1999

13th INTERNATIONAL FORUM ON PROCESS ANALYTICAL CHEMISTRY
San Antonio TX.

Information: InfoScience Services, Conference Division, 3000 Dundee Road, Suite 409, Northbrook, IL 60062, (847) 291-9161, Fax (847) 291-0097, e-mail: infoscience@ais.net, http://www.ifpac.com

JANUARY 23-29, 1999

PHOTONICS WEST
San Jose CA.

Includes International Symposia on:
- LASE'99 - High-Power Lasers and Applications
- OPTOELECTRONICS '99 - Integrated Devices and Applications
- SPIE/IS&T's EI '99 - Electronic Imaging: Science and Technology

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

FEBRUARY 6-12, 1999

PHOTONICS WEST
San Jose CA.

Information: The International Society for Optical Engineering, SPIE, Meetings Department, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, http://www.spie.org

FEBRUARY 10-12, 1999

18th IEEE INTERNATIONAL PERFORMANCE, COMPUTING AND COMMUNICATIONS CONFERENCE (IPCCC '99)
Scottsdale AZ.

Information: N. Malik, General Chairman, IBM Corporation, 11400 Burnet Road, Austin, TX 78758, (512) 838-5106, Fax (512) 838-8378, http://www.ipccc.org/ipccc99/

FEBRUARY 25-26, 1999

13th ANNUAL TECHNICAL CONFERENCE ON SOLVING ENVIRONMENTAL AND OTHER TECHNOLOGICAL CHALLENGES IN COMBUSTION FOR THE NEXT CENTURY
Provo UT.

Conference at the Advanced Combustion Engineering Research Center. Topics will Include:

- Combustion Chemistry
- NO_x /Pollutants
- Fine Particles
- Simulations/Validation

Information: Advanced Combustion Engineering Research Center, Brigham Young University, 45 CTB, Provo, UT 84602, (801) 378-4126; Fax (801) 378-3831.

FEBRUARY 28-MARCH 5, 1999

GORDON RESEARCH CONFERENCE ON GASEOUS IONS, STRUCTURE, ENERGETICS AND REACTION DYNAMICS
Ventura CA.

Organizing Chairman: T. Baer
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

FEBRUARY 28-MARCH 5, 1999

GORDON RESEARCH CONFERENCE ON CHEMICAL REACTIONS AT SURFACES
Ventura CA.

Organizing Chairman: J. Yates
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

MARCH 1-4, 1999

SAE INTERNATIONAL CONGRESS AND EXPOSITION
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

MARCH 7-12, 1999

PITTCON '99: 50th PITTSBURGH CONFERENCE ON ANALYTICAL CHEMISTRY AND APPLIED SPECTROSCOPY
Orlando FL.

Information: L. Briggs, Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (800) 825-3221, Fax (412) 925-3224.

MARCH 8-11, 1999

24th INTERNATIONAL TECHNICAL CONFERENCE ON COAL UTILIZATION AND FUEL SYSTEMS
Clearwater FL.

Information: B. Sakkestad, Coal Utilization and Fuel Systems Conference Committee, 1156 Fifteenth Street, NW, Suite 525, Washington, DC 20005, (202) 296 1133, Fax (202) 223 3504, e-mail: barbarasak@aol.com

MARCH 14-17, 1999

INTERNATIONAL FIRE SAFETY CONFERENCE
New Orleans LA.

Information: FRCA, 851 New Holland Ave., P.O. Box 3535, Lancaster, PA 17604, (717) 219-5616.

MARCH 14-18, 1999

1999 SPRING NATIONAL MEETING AND PETROCHEM EXPO OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Houston TX.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org

MARCH 15-17, 1999

TRIPLE JOINT TECHNICAL MEETING OF THE EASTERN/CENTRAL AND WESTERN STATES SECTIONS OF THE COMBUSTION INSTITUTE
Washington DC.

Information: M.D. Smooke, Becton Laboratory, Room 205, Department of Mechanical Engineering, Yale University, New Haven, CT 06520, (203) 432-4344, Fax (203) 432-6775, e-mail: mitchell.smooke@yale.edu, or
W.J. Pitz, L-14, Lawrence Livermore Laboratory, P.O. Box 808, Livermore, CA 94551, (510) 422-7730, Fax: (510) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/ or http://odie.seas.ucla.edu/WSS/, or
D. Stocker, NASA Lewis Research Center, MS 500-115, 21000 Brookpark Road, Cleveland, OH 44135, (216) 433-2166, Fax (216) 433-8660, e-mail: dennis.stocker@lerc.nasa.gov

MARCH 15-19, 1999

5th ASME/JSME THERMAL ENGINEERING CONFERENCE: THERMAL ENGINEERING FOR COMBUSTION SYSTEMS AND FIRE SAFETY
San Diego CA.

Topics will Include:
- Combustion Engines, Furnaces, Incinerators
- Combustion Synthesis, Materials Processing
- Fire Spread, Suppression
- Measurement, Modeling Methods
- Fundamental Physical Processes in Flames

Information: T. Simon, Department of Mechanical Engineering, University of Minnesota, 111 Church Street, SE, Minneapolis, MN 55455, (612) 625 5831, Fax (612) 624 5230, e-mail: tsimon@me.umn.edu, http://www.asme.org/conf/A-JSME98/index.htm

MARCH 18-19, 1999

2nd POLLUTION PREVENTION TOPICAL WORKSHOP HOSTED BY THE ENVIRONMENTAL DIVISION OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Houston TX.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org, or Contact Conference Chairman S. Butner at butner@battelle.org or J. Cramer at (212) 591-7950, e-mail: josec@aiche.org, or Program Details at http://www.seattle.battelle.org/AICHE98/

MARCH 21-25, 1999

217th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Anaheim CA.

Division of Fuel Chemistry:
- Molecular Approaches to CH Activation and Selective Oxidation of Alkanes
  R. Periana, Catalytica Advanced Technologies, 430 Ferguson Drive, Building 3, Mountain View, CA 94043-5272, (650) 940-6396, Fax (650) 968-7129, e-mail: rap@mv.catalytica-

inc.com; R.H. Crabtree, Department of Chemistry, Yale University, 225 Prospect Street, New Haven, CT 06520-8107, (203) 432-3925, Fax (203) 432-6144, e-mail: crabtree@minerva.cis.yale.edu

- Renewable Fuels and Chemicals
  R. Evans, National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, CO 80401-3393, (303) 384-6284, e-mail: evansb@tcplink.nrel.gov
- Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion
  J.A. Franz; M.T. Klein, Department of Chemical Engineering, University of Delaware, Newark, DE 19716
- New Catalysts for Hydrogenation and Hydrocracking of Fuels
  M.E. Davis, California Institute of Technology, Pasadena, CA 91125, (818) 395-6811, e-mail: mdavis@macpost.caltech.edu; S. Zones, Chevron, (510) 242-3524
- Role of Water in Organic Reactions
  M. Lewan, U.S. Geological Survey, Box 25046 MS 977, Denver Federal Center, Denver, CO 80255, (303) 236-9391, e-mail: mlewan@bpgsvr.cr.usgs.gov; G.D. Cody, Geophysical Laboratory, Institute of Washington, 5251 Broad Branch Road, N.W., Washington, DC 20015, (202) 686-2410 ext. 2479, e-mail: cody@gl.ciw.edu

Division of Petroleum Chemistry:

- Lower Alkane Oxidation
  U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu

Division of Physical Chemistry:

- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley, CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu
- Atmospheric Chemistry
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu
- Unimolecular Reactions and Intramolecular Dynamics
  S.J. Klippenstein, Chemistry Department, Case Western Reserve University, Cleveland, OH 44106, e-mail: sjk5@po.cwru.edu

Complete Information at http://www.acs.org/meetings/ anaheim/welcome.htm

MARCH 21-26, 1999

23rd ENGINEERING FOUNDATION CONFERENCE ON STATIONARY SOURCE SAMPLING AND ANALYSIS FOR AIR POLLUTANTS
Ventura CA.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

MARCH 22-26, 1999

AMERICAN PHYSICAL SOCIETY CENTENNIAL MEETING
Atlanta GA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, Fax (301) 209-0866, e-mail: meetings@aps.org

MARCH 25-26, 1999

ADVANCED MARINE MACHINERY SYSTEMS WITH LOW POLLUTION AND HIGH EFFICIENCY
Newcastle upon Tyne, UK.

Information: A. Evripidou, The Institute of Marine Engineers, 76 Mark Lane, London EC3R 7JN, UK, (171) 481-8493, Fax (171) 488 1854, e-mail: ae@imare.org.uk

MARCH 29-APRIL 2, 1999

FRONTIERS IN SCIENCE AND TECHNOLOGY: SCIENCE OF CLIMATE
La Jolla CA.

Information: Frontier Scientific Research Conference, La Jolla International School of Science, Institute for Advanced Physical Studies, 7596 Eads Ave., La Jolla, CA 92038, e-mail:wisdom@stefan-university.edu

APRIL 7-9, 1999

10th ANNUAL UNITED STATES HYDROGEN MEETING OF THE NATIONAL HYDROGEN ASSOCIATION
Vienna VA.

Information: National Hydrogen Association, 1800 M Street, N.W., Suite 300, Washington DC, 20036, (202) 223-5547.

APRIL 9-10, 1999

NEW ENGLAND SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Yale University, New Haven CT.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 11-14, 1999

13th TOPICAL CONFERENCE ON APPLICATIONS OF RADIOFREQUENCY POWER PLASMAS
Annapolis MD.

Information: S. Bernabei, Princeton Plasma Physical Laboratory, P.O. Box 451, Princeton, NJ 08543, e-mail: sbernabei@pppl.gov

APRIL 11-14, 1999

ASME CONFERENCE ON RENEWABLE AND ADVANCED ENERGY SYSTEMS FOR THE 21st CENTURY
Lahaina, Maui HI.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

APRIL 12-15, 1999

40th AIAA/ASME/ASCE/AHS/ASC STRUCTURES, STRUCTURAL DYNAMICS AND MATERIALS CONFERENCE
St. Louis MO.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

APRIL 13-16, 1999

13th INTERNATIONAL CONFERENCE ON OPTICAL FIBER SENSORS
Kyongju, South Korea.

Information: OFS-13 Secretariat, Department of Physics, KAIST, 373-1 Kusong-dong, Yusong-gu, Taejon 305-701, South Korea, e-mail: ejsohn@cais.kaist.ac.kr

APRIL 14, 1999

JOINT MEETING OF THE BRITISH SECTION OF THE COMBUSTION INSTITUTE AND UKELG: INDUSTRIAL COMBUSTION HAZARDS

Information: J. Griffiths, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK, 011-44(1132) 336462, Fax (1132) 336565.

APRIL 14-15, 1999

THE UK COAL RESEARCH FORUM ANNUAL MEETING
London UK.

Will Include Workshops on
- Fundamental Coal Research
- Conventional and Advanced Power Generation

Information: D.J.A. McCaffrey, CRE Group Ltd., Stoke Orchard, Cheltenham, Gloucester GL52 4RZ, UK, (1242) 673361, Fax (1242) 677010.

APRIL 14-16, 1999

4th INTERNATIONAL MEETING ON CATALYTIC COMBUSTION
San Diego CA.

Information: http://www.catalytica-inc.com/WCC4

APRIL 19-22, 1999

CHAPMAN CONFERENCE ON ATMOSPHERIC SCIENCE ACROSS THE STRATOSPHERE
Annapolis MD.

Information: American Geophysical Union, 2000 Florida Avenue N.W., Washington, DC 20009, (202) 462-6900, (800) 966-2481, Fax (202) 328-0566, Service and Information Center: service@agu.org, http://www.agu.org

APRIL 19-23, 1999

2nd INTERNATIONAL SYMPOSIUM ON HEAT AND MASS TRANSFER UNDER PLASMA CONDITIONS: PLASMA '99
Antalya, Turkey.

Topics will Include:

- Turbulence Phenomena in Thermal Plasmas
- Plasma Transport Properties of Complex Mixtures Including Diffusion
- Radiative Transport under Plasma Conditions
- Non-equilibrium Effects in Thermal Plasma Systems
- Plasma-Wall Boundary Layers and Electrode Erosion Phenomena
- Electromagnetically Induced Flow Effects in Plasma Systems
- Plasma Particulate Interactions
- Transport Processes in Dusty Plasmas
- Rapid Solidification During Plasma Deposition
- Particle Nucleation and Growth in Plasma Reactors
- Waste Treatments and On-line Controls in Connection with Environmental Regulations
- Material Behavior under Extremely High Heat Fluxes ($>10^9$ Wm^{-2})
- Flash Evaporation
- Diagnostic Techniques in Plasma Chemical Applications, in Dusty Plasmas, in Particle Flattening and Splat Cooling
- On-line Control in Plasma Processes
- New Branches of Plasma Physics and Transport Phenomena (MAD, Improved MHD, EHD, DL and DL Currents)

Information: P. Fauchais, Faculte des Sciences, Universite de Limoges, 123 Avenue A. Thomas, 87060 Limoges Cedex-France, (33-5) 55 45 74 21, Fax (33-5) 55 45 72 11, e-mail: fauchais@unilim.fr, or F. Arinc, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210 5214, Fax (90) 312-210 1331, e-mail: arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr
Deadline: 4-Copies of Extended Abstract to P. Fauchais (above) by October 15, 1998, Abstracts for Poster Presentations by January 30, 1999.

APRIL 23-24, 1999

NEW YORK SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Murray Hill NJ.

Information: R.S. Galik, Vice Chair, 108 Newman Laboratory, Cornell University, Ithaca, NY 14853, (607) 255 3633, Fax (607) 254 4552, e-mail: rsg@ins62.ins.cornell.edu

APRIL 25-28, 1999

ASME SPRING ENGINE TECHNOLOGY CONFERENCE ON THE INTERNAL COMBUSTION ENGINE
Columbus IN.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

APRIL 25-30, 1999

CORROSION '99: 54th NACE INTERNATIONAL CONFERENCE AND EXHIBITION
San Antonio TX.

Information: Meetings Department, NACE, P.O. Box 218340, Houston, TX 77084, (281) 228-6223, Fax (281) 228-6300, e-mail: msd@mail.nace.org, http://www.nace.org

APRIL 26-30, 1999

FRONTIERS IN SCIENCE AND TECHNOLOGY: AEROSOL SCIENCE AND TECHNOLOGY
La Jolla CA.

Information: Frontier Scientific Research Conference, La Jolla International School of Science, Institute for Advanced Physical Studies, 7596 Eads Ave., La Jolla, CA 92038, e-mail:wisdom@stefan-university.edu

APRIL 27-29, 1999

9th ANNUAL MEETING OF THE HALON OPTIONS TECHNICAL WORKING CONFERENCE
Albuquerque NM.

Topics will Include:

- Halon Replacements and Alternatives
- Advanced Technologies
- Toxicity Issues
- Halon Bank Management and Destruction
- Fire Suppression Testing
- Regulatory and Environmental Issues
- Inert Gases
- Advanced Agents
- Agent Decomposition
- Laboratory Testing
- Misting Technologies
- Particulate Aerosols
- Basic Research

Special Sessions are Planned on:

- CF_3I
- Bromoalkane Blends
- Next-Generation Fire Suppression Technology Program
- Informed Decisions: A User's Perspective

Information: R.E. Tapscott, Director, Center for Global Environmental Technologies, University of New Mexico, 901 University Boulevard SE, Albuquerque, NM 87106, (505) 272-7252, Fax (505) 222-8230, e-mail: tapscott@nmeri.unm.edu

APRIL 30-MAY 1, 1999

OHIO SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Flint, MI.

Information: Bahram Roughani, e-mail: broughan@nova.gmi.edu

MAY 2-5, 1999

4th ITALIAN CONFERENCE ON CHEMICAL AND PROCESS ENGINEERING
Florence, Italy.

Information: AUDIC ICheaP-4 Secretariat, Piazza Morandi 2, 20121 Milano, Italy, (02) 760-21175, Fax (02) 799644, e-mail: aidic@aidic.it, Web Site: http://www.aidic.it

MAY 2-7, 1999

195th MEETING OF THE ELECTROCHEMICAL SOCIETY
Seattle WA.

Symposia Include among Others:
- General Session on Corrosion
- Fullerenes: Chemistry, Physic s and New Directions

Information: http://www.electrochem.org/meetings

MAY 3-6, 1999

INTERNATIONAL FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Dearborn MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

MAY 4-7, 1999

5th ASIAN CONFERENCE ON ANALYTICAL SCIENCES
Xiamen, China.

Information: Sun Dahai, Department of Chemistry, Xiamen University, Xiamen 361005, China, Fax 86(592) 218 6401, e-mail:asianalysis@xmu.edu.cn, Web Site: http://www.xmu.edu.cn/sedc/english/confer.htm

MAY 9-12, 1999

2nd ASIA-PACIFIC CONFERENCE ON COMBUSTION
Tainan, Taiwan

Topics will Include:
- Gaseous Combustion
- Liquid Fuels, Droplet and Spray Combustion
- Solid Fuels and Coal Combustion
- Reaction Kinetics of Combustion, Pollutant formation and Control
- Laminar Flame Combustion
- Turbulent Premixed, Partially Premixed and Non-Premixed Combustion
- Detonations and Supersonic Combustion
- Internal Combustion Engines, Gas Turbine Engines and Rocket Engines
- Stationary Combustion Systems and Incineration
- Fire Research

- Material Synthesis and Catalytic Combustion Manufacturing
- Combustion Modeling and Computational Combustion
- Combustion in Microgravity Systems

Information: T.-H. Lin, Department of Mechanical Engineering, National Cheng Kung University, 1 Ta-Shue Road, Tainan, Taiwan 701, 886(6)2757575, ext. 62167, Fax 886(6)2352973, e-mail: thlin@mail.ncku,edu.tw

MAY 10-12, 1999

21st INTERNATIONAL POWER SOURCES SYMPOSIUM
Brighton UK.

Information: R.D. Bailey, Crundalls, Gedges Hill, Matfield, Kent TN12 7EA, UK, (44)1892 723408, Fax (44)1892 723874, e-mail: ipss@marketdevelopco.demon.co.uk

MAY 10-14, 1999

THE 1999 INTERNATIONAL CONFERENCE ON INCINERATION AND THERMAL TREATMENT TECHNOLOGIES
Orlando FL.

Information: Conference Coordinator, L.B. Cohen, University of California, EH&S, 300 University Tower, Irvine, CA 92697, (949) 824-5859, Fax (949) 824-1900, e-mail: lbarnow@uci.edu

MAY 16-19, 1999

ASME FLUIDIZED BED COMBUSTION CONFERENCE
Savannah GA.

Information: Meetings Department, ASME, 345 E. 47th St., New York, NY 10017, (212) 705-7037, Fax (212) 705-7143.

MAY 16-19, 1999

2nd PACIFIC SYMPOSIUM ON FLOW VISUALIZATION AND IMAGE PROCESSING
Honolulu HI.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7284, Fax (212) 705-7143, http://www.asme.org

MAY 17-19, 1999

7th ASME ANNUAL NORTH AMERICAN WASTE-TO-ENERGY CONFERENCE
Tampa FL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

MAY 17-19, 1999

32nd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Madison NJ.

Information: G. Heinz, 30 Bunker Hill Run, East Brunswick, NJ 08816, (732) 257 5754.

MAY 18-20, 1999

THE 5th INTERNATIONAL MICROGRAVITY COMBUSTION WORKSHOP
Cleveland OH.

Information: A. Heyward, Outreach Programs Manager, National Center for Microgravity Research on Fluids and Combustion, NASA Lewis Research Center, Cleveland OH, (216) 433-8173, e-mail: Ann.O.Heyward@lerc.nasa.gov, http://www.ncmr.org/events/workshop.html

MAY 18-21, 1999

JOINT MEETING OF THE BRITISH, GERMAN AND FRENCH SECTIONS OF THE COMBUSTION INSTITUTE
Nancy, France.

Information: C. Poulain (CPIC), 33(0)383301161, Fax 33(0)383175215, e-mail: cpic@ensic.u-nancy.fr

MAY 21-22, 1999

1st MEETING OF THE NORTHWEST SECTION OF THE AMERICAN PHYSICAL SOCIETY
Vancouver BC, Canada.

Information: E. Henley, e-mail: henley@nucthy.phys.washington.edu

MAY 23-25, 1999

2nd INTERNATIONAL SYMPOSIUM ON TWO PHASE FLOW MODELING AND EXPERIMENTATION
Pisa, Italy.

Information: R.K. Shah, Symposium Co-Chairman, Department of Mechanical Engineering, University of Kentucky, Lexington, KY 40506, (606) 257-6043, Fax (606) 257-3304, e-mail: shah@engr.uky.edu, or
P. Di Marco, Symposium Secretary, University of Pisa, Energy Department, Via Diotisalvi 2, I-56126 Pisa, Italy, (39) 50-569-610, Fax (39) 50-569-666, e-mail: p.dimarco@ccii.unipi.it, or see http://docenti.ing.unipi.it/d6600/pisa99/

MAY 23-28, 1999

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO 99) AND THE QUANTUM ELECTRONICS AND LASER SCIENCE CONFERENCE (QELS 99)
Baltimore MD.

Information: Information: Meetings Department, Optical Society of America, 201 Massachusetts Avenue, Washington, DC 20036, (202) 223-8130.

MAY 25-28, 1999

COMBUSTION CANADA '99: COMBUSTION AND GLOBAL CLIMATE CHANGE. CANADA'S CHALLENGES AND SOLUTIONS
Calgary, Alberta, Canada.

Topics will Include:

- Market and Technology Assessments for Greenhouse Gas Reductions
- How Electric Utilities can Succeed in the Climate Change Challenge
- Industrial Combustion and Greenhouse Gases: The Consequences and the Challenges
- More Efficient Residential and Commercial Combustion Systems
- CO_2 Capture and Sequestration
- The District Energy Solution and Climate Protection
- Flaring
- Improving Transportation Engines, Systems and Fuels for Greenhouse Gas Emission Reductions
- Biomass in Canada's Energy Mix

Information: Conference Secretariat, CC'99 Coordinator, Suite 208, 350 Sparks St., Ottawa, Ontario, Canada K1R 7S8, (613) 236-6222, Fax (613) 236-6850, e-mail: info@ceia-acie.ca, http://www.combustion-net.com

MAY 30-JUNE 2, 1999

82nd CANADIAN SOCIETY FOR CHEMISTRY CONFERENCE AND EXHIBITION
Toronto, Canada.

Information: P. Sundar Sundararajan, Xerox Research Center of Canada, 2660 Speakman Drive, Mississauga, Ontario L5K 2L1, Canada, (905) 823-7091 ext. 219, e-mail:Sundar.Sundararajan@crt.xerox.com

JUNE 6-10, 1999

5th INTERNATIONAL CONFERENCE ON CHEMICAL STRUCTURES
Noordwijkerhout, The Netherlands.

Information: G. Grethe, c/o MDL Information Systems Inc., 14600 Catalina Street, San Leandro, CA 94577, (510) 895-1313 ext. 1430, Fax (510) 614-3638, e-mail:guenter@mdli.com

JUNE 6-11, 1999

GORDON RESEARCH CONFERENCE ON OSCILLATIONS AND DYNAMIC INSTABILITIES IN CHEMICAL SYSTEMS
Il Ciocco, Italy.

Organizing Chairperson: R. Larter
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JUNE 7-8, 1999

SPQ-99: SPECTROSCOPY IN PROCESS AND QUALITY CONTROL
East Brunswick NJ.

Information: R. Vallari, Advanstar Communications, 101 Fieldcrest Avenue, Raritan Plaza III, Edison, NJ 08837, (732) 225-9500, Fax (732) 225-0211, e-mail: rvallari@advanstar.com

JUNE 7-10, 1999

ASME TURBO EXPO '99: LAND, SEA AND AIR, 44th ASME INTERNATIONAL GAS TURBINE AND AEROENGINE TECHNICAL CONGRESS EXPOSITION AND USERS SYMPOSIUM
Indianapolis IN.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

JUNE 7-11, 1999

14th INTERNATIONAL CONFERENCE ON LASER SPECTROSCOPY ICOLS '99
Innsbruck, Austria.

Topics will Include:

- Atomic and Molecular Laser Spectroscopy
- Precision Spectroscopy
- Laser Cooling and Trapping
- Quantum Optics
- Matter Wave Optics and Interferometry
- Nonlinear Optics and Spectroscopy
- Ultrafast and Strong Field Phenomena
- New Laser Sources
- Applications of Laser Spectroscopy
- Bose-Einstein Condensation and Atom Lasers

Information: D. Leibfried, Institut f. Experimentalphysik, Universitaet Innsbruck, Technikerstrasse 25, A-6020 Innsbruck, Austria, Fax (43) 512-507-2952, e-mail: icols99@uibk,ac.at, http://physics.uibk.ac.at/ICOLS99

JUNE 13-18, 1999

GORDON RESEARCH CONFERENCE ON ATMOSPHERIC CHEMISTRY
Salve Regina University, Newport RI.

Organizing Chairpersons: W.H. Brune and J.E. Penner
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JUNE 13-18, 1999

47th CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS
Dallas TX.

Information: J. Sjoberg, American Society for Mass Spectrometry, 1201 Don Diego Avenue, Santa Fe, NM 87505, (505) 989-4517, Fax (505) 989-1073, e-mail: asms@asms.org

JUNE 14-18, 1999

LASER '99
Munich, Germany.

Information: Messe Munchen GmbH, Messegelande, D-80325 Munchen, Germany, 49(0) 89 51 070, Fax 49(0) 89 51 07 506, e-mail: info@messe-muenchen.de

JUNE 15-16, 1999

FEDERAL ENERGY TECHNOLOGY CENTER/US DEPARTMENT OF ENERGY WORKSHOP ON RESPONSIBLE POWER PRODUCTION IN THE NEXT CENTURY
Arlington VA.

Focus Areas will Include:

- Why Coal - It's the Genesis of Coal-Fired Electricity Production
- Coal and Natural Gas Need Not be in Competition
- Future of Pulverized Coal Combustion as a Power Producing Choice
- Environmental Challenges for Pulverized Coal, CO_2, HAPS, Hg, $PM_{2.5}$, etc.
- Biomass Cofiring
- DOE's High Performance Power System (HIPPS) and Low Emission Boiler System (LEBS) Development Programs
- Repowering/Life Extension using HIPPS and LEBS
- Power Needs for Developing Countries
- Advanced Combined Cycles
- DOE's Vision 21 Program

Information: A.C. Bose, Federal Energy Technology Center, US Department of Energy, P.O. Box 10940, Pittsburgh, PA 15236, (412) 892-4467/4867, e-mail: bose@fete.doe.gov, http://www.fetc.doe.gov under Upcoming Events.

JUNE 16-20, 1999

4th INTERNATIONAL CONFERENCE ON DISSOCIATIVE RECOMBINATION
Stockholm, Sweden.

Information: M. Larsson, Department of Physics, Stockholm University, Box 6730, S-11385 Stockholm, Sweden, e-mail: mats.larsson@physto.se

JUNE 17-JULY 1, 1999

ADVANCES IN ENERGY TRANSFER PROCESSES: AN ADVANCED STUDY INSTITUTE
Erice, Sicily, Italy.

Information: B. Di Bartolo, Department of Physics, Boston College, Chestnut Hill, MA 02167, (617) 552-3601, Fax (617) 552-8478, http://www.ccsem.infn.it

JUNE 19-23, 1999

MEDITERRANEAN COMBUSTION SYMPOSIUM OF THE COMBUSTION INSTITUTE AND THE INTERNATIONAL CENTER FOR HEAT AND MASS TRANSFER
Antalya, Turkey.

Topics will Include:
- Stationary Sprays and Gas Combustion Systems
- Combustion of Solid Fuels PF, FBC and Waste
- Internal Combustion Engines
- Optical Diagnostics and Radiative Transfer
- Flame Dynamics and Turbulence
- Pollutants
- Fire/Explosions
- Kinetics

Information: F. Arinc, Secretary General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210 1429, Fax (90) 312-210 1331, e-mail: arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

Deadline: Submit Camera Ready Copy of the Full Paper together with Three Additional Copies, Plus One 3.5" Floppy Disk Containing in a Word File only the Title, Authors, Affiliation and Abstract by November 1, 1998 to Martine van Hapert, Istituto di Richerche sulla Combustione - CNR, P.le Tecchio, 80, 80125 Napoli, Italy, (39) 81-768 2263, Fax (39) 81-593 6936, e-mail: martine@irc.na.cnr.it

Work in Progress Presentations: Send One Camera Ready Abstract and 2-Copies by February 1, 1999 to Filiz Ozler, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210 5213, Fax (90) 312-210 1331, e-mail: ichmt@metu.edu.tr

JUNE 20-22, 1999

54th NORTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Portland OR.

Information: T. Dunne, 3203 Southeast Woodstock Boulevard, Portland, OR 97202, (503) 777-7207, Fax (503) 777-7769.

JUNE 20-24, 1999

35th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE AND EXHIBIT
Los Angeles CA.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JUNE 20-25, 1999

GORDON RESEARCH CONFERENCE ON LASER DIAGNOSTICS FOR COMBUSTION RESEARCH
Il Ciocco, Italy.

Organizing Chairpersons: K. Kohse-Hoinghaus and J.B. Jeffries
Information: J.B. Jeffries, SRI International, Molecular Physics Laboratory, 333 Ravenswood Avenue, Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: jeffries@mplvax.sri.com, http://pc1.chemie.uni-bielefeld.de/gordon
Deadline: Posters, February 15, 1999.

JUNE 21-23, 1999

31st CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Columbus OH.

Information: J. Parson, Chemistry Department, Ohio State University, 100 W. 18th Avenue, Columbus, OH 43210, (614) 292-3267, Fax (614) 292-1685, e-mail: parson2@osu.edu

JUNE 21-24, 1999

FOURIER TRANSFORM SPECTROSCOPY: NEW METHODS AND APPLICATIONS
Santa Barbara CA.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

JUNE 21-25, 1999

COURSE ON THE FUNDAMENTALS OF INTERNAL COMBUSTION ENGINES: PERFORMANCE, EFFICIENCY AND EMISSIONS
MIT, Cambridge MA.

Organized by W.K. Cheng and J.B. Heywood
Information: Professional Institute, Room 8-201, Massachusetts Institute of Technology, Cambridge, MA 02139, (617) 253-2101, Fax (617) 253-8042, e-mail: professional-institute@mit.edu, Web Site: http://web.mit.edu/professional/summer/
Course Fee: $2250.

JUNE 21-26, 1999

28th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Potsdam NY.

Information: P. Zuman, Department of Chemistry, Potsdam University, Potsdam, NY 13699, (315) 268-2340.

JUNE 27-30, 1999

PULSED POWER CONFERENCE
Monterey CA.

Information: C. Stallings, Physics International, 2700 Merced Street, San Leandro, CA 94577, e-mail: chstallings@corp.olin.com

JUNE 27-30, 1999

6th INTERNATIONAL CONGRESS ON TOXIC COMBUSTION BYPRODUCTS
Karlsruhe, Germany.

Information: e-mail: pic22@ict.uni-karlsruhe.de, http://www.ict.uni-karlsruhe.de/pic99/
Deadline: 2-Page Abstract Due by December 31, 1998, Final Paper June 1999 and will be Published in *Combustion Science and Technology*.

JUNE 27-JULY 2, 1999

GORDON RESEARCH CONFERENCE ON GRAVITATIONAL EFFECTS IN PHYSICO-CHEMICAL SYSTEMS
New England College, Henniker NH.

Organizing Chairman: R.F. Sekerka
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JUNE 27-JULY 2, 1999

GORDON RESEARCH CONFERENCE ON PHOTOACOUSTIC AND PHOTOTHERMAL PHENOMENA
Colby-Sawyer College, New London NH.

Organizing Chairman: J. Power
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JUNE 28-JULY 1, 1999

17th APPLIED AERODYNAMICS CONFERENCE/14th AIAA COMPUTATIONAL FLUID DYNAMICS CONFERENCE/30TH AIAA FLUID DYNAMICS CONFERENCE/30TH AIAA PLASMADYNAMICS AND LASERS CONFERENCE/33RD AIAA THERMOPHYSICS CONFERENCE
Norfolk VA.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JUNE 29-JULY 1, 1999

INTERFLAM '99
Edinburgh, Scotland.

Topics will Include:
- Advances in Detection, Extinction and Suppression - Halon Replacement
- Applied Fire Safety Science and the Fire Service
- Comparison of Computer Models with Experimental Data
- Disaster Mitigation and Large Fire Studies (Forest Fires)
- Education
- Fire Behavior of Materials
- Fire Dynamics - Flame Spread and Heat Release Studies
- Fire Risk Assessment
- Harmonization of Fire Safety Standards
- Heat Transfer from Flames
- Human Behavior and Evacuation Modeling
- Interpretation of Small Scale Test Datea
- Properties of Combustion Products
- Performance Based Codes
- Structural Behavior

Information: C. Franks, Conference Secretariat, Interscience Communications Ltd., West Yard House, Guildford Grove, Greenwich, London Se10 8JT, UK, 44(181)692 5050, Fax 44(181)692 5155, e-mail: intercomm@dial.pipex.com.uk

JULY 4-6, 1999

2nd INTERNATIONAL SYMPOSIUM ON INCINERATION AND FLUE GAS TREATMENT TECHNOLOGIES
Sheffield UK.

Information: J. Black, Conference Department, IChemE, 165-189 Railway Terrace, Rugby CV21 3HQ, Warwickshire, UK, 011-44 (1788) 578214, Fax (1788) 577182, e-mail: jblack@icheme.org.uk

JULY 5-7, 1999

15th ANNUAL CONFERENCE ON LIQUID ATOMIZATION AND SPRAY SYSTEMS
Toulouse, France.

Information: Secretariat ILASS-Europe '99, ONERA-Centre de Toulouse, 2 Av. Edourd Belin, BP 4025, 31055 Toulouse Cedex, France, (5) 62 25 25 82, Fax (5) 62 25 25 83, e-mail: gerard.lavergne@onecert.fr

JULY 5-9, 1999

STEREOCHEMISTRY AND CONTROL IN MOLECULAR REACTION DYNAMICS. A DISCUSSION COMPARING FREQUENCY, TEMPORAL AND PHASE CONTROL STRATEGIES TO PROBE ELEMENTARY CHEMICAL PROCESSES: A FARADAY DISCUSSION OF THE ROYAL SOCIETY OF CHEMISTRY
Leeds, UK.

Topics will Include:
- High Resolution Studies (Both Frequency and Time Resolved) of Molecular Photodissociation or Photoinitiated Processes
- Control of Reactivity via Collision Energy, Selective Vibration of Reagents, or Reagent Alignment
- Demonstrations of Active or Coherent Control of Chemical Processes

Information: http://www.chem.leeds.ac.uk/faraday 113/

JULY 5-9, 1999

6th INTERNATIONAL SYMPOSIUM ON FIRE SAFETY SCIENCE
Poitiers, France.

Topics will Include:
- Fire Physics
- Fire Chemistry
- Smoke and Toxic Hazard
- Fire Behavior of Materials
- Stochastic Modeling and Risk Assessment
- Human Behavior and Egress
- Fire Spread
- External Fires
- Structural Behavior
- Fire Detection and Suppression
- Advanced Applications of Fire Safety Science
- Specialized topics in Fire Safety and Protection

Information: 6th IAFSS Symposium Organizers, LCD-ENSMA, Teleport 2, B.P. 109-86960 Futuroscope Cedex, France, 33(0)5 49 49 82 90, Fax 33(0)5 49 49 82 91, e-mail: iafss6@lcd.ensma.fr

JULY 11-15, 1999

NATIONAL CONFERENCE OF STANDARDS LABORATORIES: ANNUAL WORKSHOP AND SYMPOSIUM
Charlotte NC.

Information: D. Nebel, e-mail: denebel@aol.com or http://www.ncsl-hq.org

JULY 11-16, 1999

GORDON RESEARCH CONFERENCE ON THE CHEMISTRY AND PHYSICS OF THE DYNAMICS OF SIMPLE SYSTEMS
Salve Regina University, Newport RI.

Organizing Chairman: C. Chandler
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JULY 11-16, 1999

GORDON RESEARCH CONFERENCE ON FREE RADICAL REACTIONS
Holderness School, Plymouth NH.

Organizing Chairman: D.P. Curran
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JULY 11-16, 1999

GORDON RESEARCH CONFERENCE ON THE PHYSICS AND CHEMISTRY OF MATRIX ISOLATED SPECIES
Plymouth State College, Plymouth NH.

Organizing Chairman: B. Ault
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JULY 12-15, 1999

CLEAN AIR V: 5th INTERNATIONAL CONFERENCE ON TECHNOLOGIES AND COMBUSTION FOR A CLEAN ENVIRONMENT
Lisbon, Portugal.

Information: Maria da Graca Carvalho, Mechanical Engineering Department, Instituto Superior Tecnico, Av Rovisco Pais, 1096 Lisbon Codex, Portugal, 351 (1) 841 7372 or 7186, Fax 351 (1) 847 5545 or (1) 726 2633, e-mail: cleanair@esoterica.pt

JULY 12-16, 1999

24th INTERNATIONAL CONFERENCE ON PHENOMENA IN IONIZED GASES
Warsaw, Poland.

Information: J. Wolowski, Institute of Plasma Physics and Laser Microfusion, 23 Hery St., P.O. Box 49, 00-908 Warsaw, Poland, e-mail: icpig99@ifpilm.waw.pl

JULY 13-15, 1999

6th INTERNATIONAL WORKSHOP ON FEMTOSECOND TECHNOLOGY
Chiba, Japan.

Information: FST'99 Secretariat, The Femtosecond Technology Research Association, 5-5 Tokodai, Tsukuba 300-2635, Japan, (81) 298-47-5181, Fax (81) 298-47-4417, e-mail: fst@festa.or.jp, http://www.festa.or.jp

JULY 18-23, 1999

THE 1999 DYNAMICS OF MOLECULAR COLLISIONS CONFERENCE
Lake Harmony PA.

Information: J.J. Valentini, Department of Chemistry, Columbia University, New York, NY 10027, (212) 854-7590, e-mail: Bitnet,VA1Valentini@cuchem

JULY 18-23, 1999

GORDON RESEARCH CONFERENCE ON ENERGETIC MATERIALS
Queen's College, Oxford UK.

Organizing Chairman: P.J. Haskins
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JULY 18-23, 1999

GORDON RESEARCH CONFERENCE ON PHOTOIONS, PHOTOIONIZATION AND PHOTODETACHMENT
Plymouth State College, Plymouth NH.

Organizing Chairman: E. Poliakoff
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JULY 18-23, 1999

SPIE ANNUAL MEETING
Denver CO.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 18-23, 1999

ASME/JSME FLUIDS ENGINEERING CONFERENCE
San Francisco CA.

Symposium Programs Include:

- Industrial Applications of Swirling Flows, Organizer, M. Padmanabhan, Alden Research Laboratory, 30 Shrewsbury St., Holden, MA 01520, (508) 829-6000, Fax (508) 829-5939, e-mail: Padu@aldenlab.com
- Numerical Developments in CFD, Organizer, M. Dhaubhadel, Ford Motor Company, (313) 248-5501, (313) 322-1733, e-mail: Mdhaubha@ford.com
- 8th International Symposium on Gas/Particle Flows, Organizer, D. Stock, Washington State University, Pullman, WA 99164, (509) 335-3223, Fax (509) 335-4662, e-mail: stock@mme.wsu.edu
- Turbulent Mixing and Diffusion, Organizers, J.C. Hill, Iowa State University, and K. Ghia, University of Cincinnati.
- Thermal Anemometry, Organizers, J. Foss, Michigan State University, East Lansing, MI 48824, (517) 355-3337, Fax (517) 353-5547, e-mail: Foss@msu.egr, or O.F. Turan, e-mail: Ofturan@dingo.vut.edu.au
- Experimental and Numerical Flow Visualization and Laser Anemometry, Organizer, B. Kahlighi, GM Research & Development, Warren, MI 48090, (810) 986-0885, Fax (810) 986-0918, e-mail: Bkhaligh@cmsa.grm.com
- Finite Element Applications in Fluid Mechanics, Organizer, M. Dhaubhadel, Ford Motor Company, 2000 Rotunda Dr., Dearborn, MI 48121, (313) 248-5501, Fax (313) 322-1733, e-mail: Mdhaubha@ford.com
- Shock Waves and Compressible Flows, Organizers, M. Morris, Bradley University, O. Baysal, Old Dominion University, and A. Kuhl, Lawrence Livermore.
- Optical Methods and Image Processing in Fluid Mechanics, Organizer, R.J. Adrian, University of Illinois, Department of Theoretical and Applied Mechanics, University of Illinois, 216 Talbot Laboratory, 104 S. Wright St., Urbana, IL 61801, (217) 333-1793, Fax (217) 244-5707, e-mail: r-adrian@uiuc.edu

JULY 19-23, 1999

5th INTERNATIONAL CONFERENCE ON LASER ABLATION, COLA '99
Goettingen, Germany.

Information: M. Stuke, Co-Chair COLA 99, e-mail: mstuke@gwdg.de, http://www.mpibpc.gwdg.de/COLA_99/

JULY 22-27, 1999

21st INTERNATIONAL CONFERENCE ON THE PHYSICS OF ELECTRONIC AND ATOMIC COLLISIONS, ICPEAC '99
Sendai, Japan.

Information: M. Matsuzawa, Applied Physics and Chemistry, University of Electro-Communications, Tokyo, 182-8585, Japan, e-mail: michio@pc.uec.ac.jp, http://power1.pc.uec.ac.jp/sendai

JULY 25-28, 1999

INTERNATIONAL JOINT POWER GENERATION CONFERENCE AND EXPOSITION
Burlingame CA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7793, Fax (212) 705-7143, http://www.asme.org

JULY 25-30, 1999

INTERNATIONAL CONFERENCE ON ANALYTICAL CHEMISTRY: ANALYTICAL SCIENCE IN THE NEXT MILLENNIUM
Dublin, Ireland.

Information: R. Smyth, Dublin City University, Dublin 9, Ireland, (353) 1-7045-308, Fax (353) 1-7045-032, e-mail: smythm@ccmail.dcu.ie

JULY 25-30, 1999

17th INTERNATIONAL COLLOQUIUM ON THE DYNAMICS OF EXPLOSIONS AND REACTIVE SYSTEMS
Heidelberg, Germany.

Information: U. Riedel, Universitat Heidelberg, IWR, Im Neuenheimer Feld 368, D-69120 Heidelberg, Germany, 49(6221) 54 8887, Fax 49(6221) 54 8884, e-mail: icders99@iwr.uni-heidelberg.de, http://reaflow.iwr.uni-heidelberg.de/icders99.html
Deadline: Camera ready Extended Abstracts (up to 4-Pages) of Papers or Posters by December 1, 1998. Electronic Submission is Encouraged, and should be Addressed to: J. Buckmaster, 321A Talbot Laboratory, 104 S. Wright St., Urbana, IL 61801, (217) 333 1803, Fax (217) 244 0720, e-mail: icders@uiuc.edu

JULY 25-30, 1999

GORDON RESEARCH CONFERENCE ON NONLINEAR OPTICS AND LASERS
Colby-Sawyer College, New London NH.

Organizing Chairman: A. Weiner
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ AUGUST 1-5, 1999

41st ROCKY MOUNTAIN CONFERENCE ON ANALYTICAL CHEMISTRY
Denver CO.

Information: Milestone Presentations, LLC, 4255 S. Buckley Road, #118, Aurora, CO 80013, (800) 996-3233 or (303) 690-3233, e-mail: milestone@bodnet, www.milestoneshows.com/rmcac

AUGUST 1-5, 1999

16th INTERNATIONAL SYMPOSIUM ON COMBUSTION PROCESSES
Kazimierz Dolny, Poland.

Topics will Include:
- Combustion in IC Engines
- Combustion Generated Pollutants
- Combustion Diagnostics
- Combustion Chemistry and Physics
- Flames and Detonations
- Fires and Explosions
- Heterogeneous Combustion
- Practical Combustion Systems
- Mathematical Modeling in Combustion

Information: A. Kowalewicz, Radom Technical University, Institute of Maintenance of Vehicles and Machines, Al. Chrobrego 45, 26-600 Radom, Poland, Fax (48)48 440 74, e-mail: kowala@kiux.man.radom.pl
Deadline: 2 Copies of a 1-Page Abstract Due January 31, 1999.

AUGUST 1-5, 1999

34th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Vancouver, British Columbia, Canada.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

AUGUST 1-6, 1999

5th WORLD CONGRESS OF THEORETICALLY ORIENTED CHEMISTS
London, UK.

Information: J. Gibson, WATOC '99, The Royal Society of Chemistry, Burlington House, London W1V 0BN, UK, (171) 437 8656, Fax (171) 734 1227, e-mail: conferences@rsc.org

AUGUST 1-6, 1999

GORDON RESEARCH CONFERENCE ON QUANTUM CONTROL OF ATOMIC AND MOLECULAR MOTION
Plymouth State College, Plymouth NH.

Organizing Chairmen: R.J. Gordon and P. Brumer
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ AUGUST 4-6, 1999

5th UNITED STATES NATIONAL CONGRESS ON COMPUTATIONAL MECHANICS
Boulder CO.

Information: K. Willam, University of Colorado, Boulder, CO 80309, (303) 492-7011, Fax (303) 492-7317, e-mail: willam@colorado.edu, http://civil.colorado.edu/usccm99/

AUGUST 8-13, 1999

GORDON RESEARCH CONFERENCE ON DYNAMICS AT SURFACES
Proctor Academy, Andover NH.

Organizing Chairman: A. Kleyn
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

AUGUST 14-17, 1999

33rd ASME NATIONAL HEAT TRANSFER CONFERENCE
Albuquerque NM.

This Conference will Include a Symposium on Heat Transfer in Combustion and Fire. Topics will Include:

- Radiation and Heat Transfer
- Fundamentals of Combustion
- Practical Combustion
- Combustion Instrumentation and Diagnostics
- Open Forum on Combustion
- Definition of a Model Problem for Experiments and Digital Computing of Fires

Information: M. di Marzo, Mechanical Engineering Department, University of Maryland-College Park, MD, 20742, (301) 405-5257, Fax (301) 314-9477, e-mail: marino@eng.umd.edu, http://www.asme.org/conf/

AUGUST 14-19, 1999

IUPAC CONGRESS ON FRONTIERS IN CHEMISTRY
Berlin, Germany.

Information: Gesellschaft Deutscher Chemiker GDCh, P.O. Box 90 04 40, D-60444, Frankfurt am Main, Germany, 49 69 7917 358/360/366, Fax 49 69 7917 475, e-mail: tg@gdch.de

AUGUST 15-20, 1999

25th INTERNATIONAL SYMPOSIUM ON FREE RADICALS
Flagstaff AZ.

Information: T.A. Miller, The Ohio State University, Web Site: http://frs.mps.ohio-state.edu/frs

AUGUST 16-19, 1999

5th INTERNATIONAL SYMPOSIUM ON SELF-PROPAGATING HIGH TEMPERATURE SYNTHESIS
Moscow, Russia.

Information: Organizing Committee, Institute of Structural Macrokinetics and Materials Science, Russian Academy of Sciences, 7(095)962 80 08, Fax 7(095)962 80 40, e-mail: shs99@ism.ac.ru or merzh@isman0.unicon.msk.su, http://www.ism.ac.ru/SHS99.html

♦ AUGUST 16-20, 1999

MEGASYMPOSIUM: COMBINED NO_x , SO_2 , PARTICULATES AND AIR TOXICS
Atlanta GA.

Information: C. Layman, (650) 855-8763, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

AUGUST 18-21, 1999

1st INTERNATIONAL CONFERENCE ON ENGINEERING THERMOPHYSICS
Beijing, China.

Topics will Include:
- Advanced Thermodynamic Cycles and New Energy Systems
- Aerothermodynamics in Turbomachinery and Other Internal Flow Devices
- Heat and Mass Transfer and Heat Exchangers
- Combustion
- Multiphase Flow Problems
- Thermophysics Measurements
- Environmental Problems Related with Thermophsics
- All Other Related Topics

Information: Ms. H. Ke, Chinese Society of Engineering Thermophysics, P.O. Box 2706, Beijing 100080, China, (8610) 62566816, Fax (8610) 62555581, e-mail: xjz@etpserver.etp.ac.cn

AUGUST 22-26, 1999

218th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Division of Fuel Chemistry:
- Tutorial on Advanced Analytical Methods for Fossil Fuels and Products
  R.E. Winans, Chemistry Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, e-mail: rewinans@anl.gov
- Molecular and Network Structures of Coal
  M. Iino, Institute of Chemical Reaction Science, Tohoku University, Katahira 2-1-1 Aoba-Ku, Sendai 980, Sendai, Japan, e-mail: iino@icrs.tohoku.ac.jp; R.E. Winans, Chemistry Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, e-mail: rewinans@anl.gov
- Hydrogen Production, Storage, and Utilization
  C. Gregoire-Padro, National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, CO 80401, (303) 275-2919.
- Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion
  J.A. Franz, M.T. Klein, Rutgers, State University of New Jersey, College of Engineering, Office of the Dean, 98 Brett Road, Piscataway, NJ 08854, (732) 445-2214, Fax (732) 445-5313, e-mail: mtklein@email.eng.rutgers.edu
- Recent Advances in Fuel Cells
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext. 142, Fax (860) 528-0648, e-mail: marek@afrinc.com

Division of Physical Chemistry:

- Imaging in Chemical Dynamics
  A. Suits, Department of Chemistry, University of California, Berkeley, CA 94720, (510) 486-4754, Fax (510) 486-5311, e-mail: agsuits@lbl.gov; R. Continetti, Department of Chemistry and Biochemistry, University of California, 9500 Gilman Drive, La Jolla, CA 92093-0314, (619) 534-5999, Fax (619) 534-7042, e-mail: rcontinetti@ucsd.edu
- Electronically Nonadiabatic Processes in Gaseous, Cluster, and Condensed Media
  L.J. Butler, Department of Chemistry, University of Chicago, 5640 S Ellis Avenue, Chicago, IL 60637, (773) 702-7206, Fax (773) 702-5863, e-mail: ljb4@midway.uchicago.edu; D.G. Truhlar, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455, (612) 624-7555, Fax (612) 626-9390, e-mail: truhlar@umn.edu
- Water Clusters, Liquid Water, and Ice: Water in Biological Systems & Heterogeneous Atmospheric Processes
  M. Johnson, Department of Chemistry, Yale University, 225 Prospect Street, New Haven, CT 06520, (203) 432-3916, Fax (203) 432-6144, e-mail: johnson@cluster.chem.yale.edu; R. Saykally, Department of Chemistry, University of California, Berkeley CA 94720, (510) 642-8269, Fax (510) 642-8369, e-mail: saykally@cchem.berkeley.edu
- Chemical Waves, Fronts and Patterns
  J. Pojman, Department of Chemistry and Biochemistry, University of Southern Mississippi, Hattiesburg, MS 39406, (601) 266-5035, Fax (601) 266-6075, e-mail: john.pojman@usm.edu; I. Epstein, Department of Chemistry, Brandeis University, Mail stop 134, Waltham, MA 02254, (781) 736-2101, Fax (781) 736-3457, e-mail: epstein2@binah.cc.brandeis.edu; V. Volpert, Laboratoire d'analyse numirique, University Lyon I, Batiment 101, 43, bd du 11 Novembre 1918, 69622 Villeubanne Cedex, France, 33-472-448317, Fax 33-472-448053, e-mail: volpert@lan1.univ-lyon1.fr
- Modern Electronic Structure Theory: Celebrating the 1998 Nobel Prize in Chemistry
  L. Curtiss, Chemistry Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, e-mail: curtiss@anlchm.chm.anl.gov

Deadline: Four Copies of Abstract (Original on ACS Abstract Form) Due to Symposium Chair by March 15, 1999. Preprints are Due by April 15, 1999.

AUGUST 22-26, 1999

14th OZONE WORLD CONGRESS
Dearborn MI.

Information: M. Istok, IOA/PAG Executive Director, 31 Strawberry Hill Avenue, Stamford, CT 06902, (203) 348-3542, Fax (203) 967-4845, e-mail: mistok@i-2000.com, or mistok@int-ozone-assoc.org

AUGUST 23-27, 1999

12th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY
Waseda University, Tokyo, Japan.

Information: ICOFTS-12 Conference Office, c/o Koichi Itoh, General Chairman, Department of Chemistry, School of Science and Engineering, Waseda University, Shinjuku-ku, Tokyo 169, Japan, http://www.chem.waseda.ac.jp/icofts/

AUGUST 29-SEPTEMBER 3, 1999

ENGINEERING FOUNDATION CONFERENCE ON ENVIRONMENTAL TECHNOLOGY FOR OIL POLLUTION: REMEDIATION AND POLLUTION PREVENTION
Jurata, Poland.

Organizing Chairmen: J. Hupka and J. Miller
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

♦ SEPTEMBER 1-4, 1999

ELECTROTHERMAL ATOMIZATION AND VAPORIZATION TECHNIQUES IN AAS, OES AND ICP-MS
Nevsehir, Turkey.

A Pre-Symposium to the 31st Colloquium Spectroscopicum International
Information: O. Yavuz Ataman, Department of Chemistry, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-3232, Fax (90) 312-210-1280, e-mail: xxxicsi@rorqual.cc.metu.edu.tr, http://www3.itu.edu.tr/~eta/

SEPTEMBER 5-9, 1999

15th EUROPEAN CONFERENCE ON THERMOPHYSICAL PROPERTIES
Wurzburg, Germany.

Information: J. Fricke, Physikalisches Institut der Universitat, Am Hubland, D-97074 Wurzburg, Germany, e-mail: ectp@zae.uni-wuerzburg.de

SEPTEMBER 5-10, 1999

8th INTERNATIONAL SYMPOSIUM ON COMPUTATIONAL FLUID DYNAMICS
Bremen, Germany.

Information: ISCFD '99, ZARM, Universitat Bremen, Am Fallturm, D-28359 Bremen, Germany, (49) 421-218-4786, Fax (49) 421-218-2521, e-mail: iscfd99@zarm.uni-bremen.de

SEPTEMBER 5-10, 1999

14th INTERNATIONAL SYMPOSIUM ON AIRBREATHING ENGINES
Florence, Italy.

Information: F. Martelli, Department of Energetics, "S. Stecco," University of Florence, Via S. Marta, 3, I-50139 Florence, Italy, (39) 55-471-925/479-6237, Fax (39) 55-479-6342, e-mail: martelli@ing.unifit.it

SEPTEMBER 5-10, 1999

31st COLLOQUIUM SPECTROSCOPICUM INTERNATIONALE
Ankara, Turkey.

Information: O.Y. Ataman, Department of Chemistry, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-3232, Fax (90) 312-210-1280 e-mail: xxxicsi@rorqual.cc.metu.edu.tr; http://www.metu.edu.tr/~wwwcsi31

♦ SEPTEMBER 6-10, 1999

EUROPEAN AEROSOL CONFERENCE
Prague, Czech Republic.

Information: Wladyslaw W. Szymanski, University of Vienna, Institute of Experimental Physics, Boltzmanngasse 5, A-1090 Vienna, Austria.

SEPTEMBER 12-15, 1999

1st INTERNATIONAL SYMPOSIUM ON TURBULENCE AND SHEAR FLOW PHENOMENA
Santa Barbara CA.

Information: S. Banerjee, Department of Chemical Engineering, University of California at Santa Barbara, Santa Barbara, CA 93106, (805) 893 3456, Fax (805) 893 4731, e-mail: tsfp@engineering.ucsb.edu

SEPTEMBER 12-15, 1999

6th INTERNATIONAL CONFERENCE ON METHODS AND APPLICATIONS OF FLUORESCENCE SPECTROSCOPY
Paris, France.

Information: B. Valeur, MAFS6-Conservatoire National des Arts et Metiers, 292 rue Saint-Martin, F-75141 Paris Cedex 03, France, 33 01 40 27 23 89, Fax 33 01 40 27 23 62, e-mail: mafs6@cnam.fr, http://www.lbpa.ens-cachan.fr/photobm/mafs6

SEPTEMBER 12-17, 1999

10th INTERNATIONAL CONFERENCE ON COAL SCIENCES: PROSPECT FOR COAL SCIENCE IN THE 21ST CENTURY
Taiyuan, Shanxi

Topics will Include:
- Fundamentals and General Aspects
- Combustion and Conversion Science
- Chemicals and Materials from Coal
- Coal Preparation and Beneficiation
- Environment Aspects

Information: L. Zhou, 10th ICCS Secretariat, Institute of Coal Chemistry, Chinese Academy of Sciences, P.O. Box 165, Tiayuan, Shanxi, 030001, P.R. China, Phone/Fax (86) 351-4048967, e-mail: iccs99@ms.sxicc.ac.cn, http://www.sxicc.ac.cn

SEPTEMBER 12-17, 1999

BEIJING INTERNATIONAL CONFERENCE ON PHOTOELECTRON SPECTROSCOPY: MOLECULES, IONS AND CLUSTERS
Beijing, China.

Information: Z. Xingkang, e-mail: zhangxk@info3.icas.ac.cn

♦ SEPTEMBER 15-17, 1999

AIR AND WASTE MANAGEMENT ASSOCIATION INTERNATIONAL SPECIALTY CONFERENCE ON MERCURY IN THE ENVIRONMENT
Minneapolis-St. Paul MN.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

SEPTEMBER 16-18, 1999

3rd INTERNATIONAL WORKSHOP ON PARTICLE IMAGE VELOCIMETRY
Santa Barbara CA.

Topics will Include:

- Optical Systems
- Interrogation Algorithms
- Post-processing
- Data Processing
- Three-Dimensional PIV
- Photogrammetric Methods
- Doppler Global Methods
- Scalar Imaging Velocimetry
- Laser Systems for PIV
- Combined Imaging and Measurement of Velocity and Scalars
- Measurement Systems and Applications to:
  - Turbulence
  - Multiphase Flow
  - Large-scale Flow
  - Microflow
  - High Speed Flow
  - Complex Engineering Flowfields
  - Biomedical Fluid Mechanics
  - Low Gravity Fluid Mechanics
  - Combustion

Information: S. Vito, UCSB Campus Conference Services, Santa Barbara, CA 93106, (805) 893-3072, Fax (805) 893-7287, e-mail: piv99@engineering.ucsb.edu, http://www.engineering.ucsb.edu/~piv99

SEPTEMBER 17-22, 1999

PHOTONICS EAST
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

♦ SEPTEMBER 19-21, 1999

ANNUAL CONFERENCE OF THE FLORIDA SECTION OF THE AIR WASTE AND MANAGEMENT ASSOCIATION
Orlando FL.

Information: C. David Cooper, CEE Department, University of Central Florida, Orlando, FL 32816, (407) 823-2388, e-mail: cooper@mail.ucf.edu

♦ SEPTEMBER 19-22, 1999

INSTRUMENTAL METHODS OF ANALYSIS: MODERN TRENDS AND APPLICATIONS
Chalkidiki, Greece.

Information: IMA '99 Secretariat, (301) 7723098, Fax (301) 7723188, e-mail: tom1sec@orfeas.chemeng.ntua.gr, http://www.chemeng.ntua.gr/IMA99/IMA99.htm

SEPTEMBER 19-24, 1999

ENGINEERING FOUNDATION CONFERENCE ON MICROGRAVITY FLUID PHYSICS AND HEAT TRANSFER
Oahu HI.

Organizing Chairpersons: V. Dhir, J. Straub and Y. Fujita
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

SEPTEMBER 19-24, 1999

5th ENGINEERING FOUNDATION CONFERENCE ON THE CONTROL OF PARTICULATE PROCESSES
Queensland, Australia.

Organizing Chairman: J. Litster
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

♦ SEPTEMBER 22-24, 1999

AIR AND WASTE MANAGEMENT ASSOCIATION SPECIALTY CONFERENCE ON HAZARDOUS WASTE COMBUSTION
Dallas TX.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

SEPTEMBER 25-OCTOBER 1, 1999

INTERDISCIPLINARY LASER SCIENCE CONFERENCE AND THE ANNUAL MEETING OF THE OPTICAL SOCIETY OF AMERICA
Santa Clara CA.

Information: Meetings Department, Optical Society of America, 201 Massachusetts Avenue, Washington, DC 20036, (202) 223-8130.

SEPTEMBER 27-28, 1999

GAMM CONFERENCE ON NUMERICAL METHODS IN FLUID MECHANICS
Kirchzarten, Black Forest, Germany.

Information: D. Kroner, Institut fur Angewandte Mathematik, University Freiburg, D-79104 Freiburg, Germany, (49) 761-203-5637/-5640, Fax (49) 761-203-5632, e-mail: dietmar@mathematik.uni-freiburg.de

♦ SEPTEMBER 27-28, 1999

4th ANNUAL GLOBAL CLIMATE CHANGE RESEARCH SEMINAR
Columbus OH.

Information: C. Gerlach, (650) 855-8579, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

♦ SEPTEMBER 28-30, 1999

ANNUAL MEETING OF THE SOUTH ATLANTIC STATES SECTION OF THE AIR WASTE AND MANAGEMENT ASSOCIATION
Virginia Beach VA.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org, or D. Trenholm, (919) 851-8181, ext. 5144.

♦ SEPTEMBER 28-30, 1999

SAE SMALL ENGINE TECHNOLOGY CONFERENCE AND EXPOSITION
Madison WI.

Information: Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org, or K. Bolcshazy, e-mail: karinb@sae.org

OCTOBER 1-2, 1999

4 CORNERS SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Tucson AZ.

Information: J.D. Garcia, e-mail: jdg@physics.arizona.edu, or American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 4-8, 1999

FULLERENES AND ATOMIC CLUSTERS
St. Petersburg, Russia.

Information: e-mail: fuller@vul.ioffe.rssi.ru, Web Site: http://www.ioffe.rssi.ru/IWFAC99/index.html

OCTOBER 5-8, 1999

GASEOUS ELECTRONICS CONFERENCE
Norfolk VA.

Information: L. Vuskovic, Old Dominion University, e-mail: lxv100f@oduvm.cc.odu.edu

OCTOBER 6-9, 1999

35th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ontario CA.

Information: V.L. Barrett, Sunkist Growers, 760 East Sunkist Street, Ontario, CA 91761, (909) 933 2291, Fax (909) 933 2453, e-mail: vbarrett@isdnt.sunkist-ppd.com

OCTOBER 8-9, 1999

OHIO SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
AFIT and Wright State University, OH.

Information: R. Hengehold, e-mail: rhengeho@afit.af.mil, or American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ OCTOBER 11-13, 1999

EASTERN STATES SECTION MEETING OF THE COMBUSTION INSTITUTE: CHEMICAL AND PHYSICAL PROCESSES IN COMBUSTION
Raleigh NC.

Invited Papers will Include:

- "Flow Dynamics of Buoyant Plumes and Diffusion Flames," Baki M. Cetegen, University of Connecticut
- "Computations of Turbulent Combustion with Detailed Chemistry," Stephen B. Pope, Cornell University
- "Combustion 2000 - Burning Coal in the 21st Century," Daniel J. Seery, United Technologies Research Center
- "Ether Additives for Reduced Diesel PM: Chemistry and Vehicle Emissions," M. Matti Maricq, Ford Motor Company
- "Chemical Fire Suppressants: How Can We Replace Halon?," James W. Fleming, Naval Research Laboratory

Information: William M. Pitts, 100 Bureau Drive, Mail Stop 8653, Bldg. 224, Room B360, National Institute of Standards and Technology, Gaithersburg, MD 20899, (301) 975-6486, Fax (301) 975-4052, e-mail: wpitts@nist.gov, http://www.ecs.umass.edu/ESSCI

♦ OCTOBER 16-20, 1999

ASME INTERNAL COMBUSTION ENGINE DIVISION FALL TECHNICAL CONFERENCE
Ann Arbor MI.

Information: Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

OCTOBER 17-20, 1999

51st SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Knoxville TN.

Information: C. Feigerle, University of Tennessee, Department of Chemistry, Knoxville, TN 37996, (615) 974-2129, e-mail: reglmtgs@acs.org

♦ OCTOBER 17-20, 1999

GASIFICATION TECHNOLOGIES CONFERENCE
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

OCTOBER 17-22, 1999

JOINT INTERNATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Honolulu HI.

Topics will Include:
- Corrosion
- Plasma Etching Processes
- Diamond Formation and Materials
- Fullerenes
- Fuel Cells

Information: http://www.electrochem.org/meetings
Deadline: Abstracts Due by May 14, 1999.

OCTOBER 21-23, 1999

JOINT 55th SOUTHWEST/15th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
El Paso, TX.

Information: K. Pannell, Chemistry Department, University of Texas, El Paso, TX 79968, (915) 747 5796, Fax (915) 747 5748 e-mail: kpannel@utep.edu

OCTOBER 24-27, 1999

FIRE RETARDANT CHEMICAL ASSOCIATION MEETING
New Orleans LA.

Information: FRCA, 851 New Holland Avenue, P.O. Box 3535, Lancaster, PA 17604, (717) 219-5616.

OCTOBER 24-28, 1999

6th ENGINEERING FOUNDATION CONFERENCE ON THE PRESENT AND FUTURE ENGINES FOR AUTOMOBILES
Orvieto, Italy.

Organizing Chairman: R. Rinolfi, T. Kamimoto and D. Foster
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

OCTOBER 24-29, 1999

26th ANNUAL CONFERENCE OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Vancouver, British Columbia, Canada.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, http://FACSS.org/info.html

♦ OCTOBER 25-26, 1999

FALL MEETING OF THE WESTERN STATES SECTION OF THE COMBUSTION INSTITUTE
Irvine CA.

Invited Papers will Include:

- "Will Fuel Cells Replace Combustion?," G. Scott Samuelsen, National Fuel Cell Research Center, University of California, Irvine.
- Physiological Interactions of Inhaled Particles," R.F. Phalen, Department of Community and Environmental Medicine, University of California, Irvine.
- "Optical Diagnostics for Dummies," J.W. Daily, Department of Mechanical Engineering, University of Colorado, Boulder.
- "Aspects of Rate-Ratio Asymptotics Applied to Flames," Kalyanasundaram Seshadri, Chemical Engineering and Fluid Mechanics, Department of Applied Mechanics and Engineering Sciences, University of California, San Diego.

Information: W.J. Pitz, L-353, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/

OCTOBER 25-28, 1999

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Toronto, Ontario, Canada.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ OCTOBER 26-28, 1999

THE EMISSION INVENTORY CONFERENCE OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Raleigh NC.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

OCTOBER 27-29, 1999

34th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Quincy IL.

Information: H.D. Wohlers, Truman State University, Science Hall, 100 East Normal, Kirksville, MO63501, (816) 785 4625, Fax (816) 785 4045, e-mail: wohlers@truman.edu

OCTOBER 28-30, 1999

TEXAS SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Austin TX.

Information: C.A. Quarles, e-mail: C.Quarles@tcu.edu, or the American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 5-6, 1999

NEW ENGLAND SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Waterville ME.

Information: C. Conover, e-mail: cwconove@colby.edu, or American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 7-9, 1999

SOUTHEASTERN SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Chapel Hill NC.

Information: T. Clegg, e-mail: clegg@TUNL.tunl.DUKE.edu, or the American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 14-19, 1999

1999 ASME INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION: SYMPOSIUM ON FIRE AND COMBUSTION SYSTEMS
Nashville TN.

Topics will Include:

- Combustion in Practical Systems
- Turbulence/Radiation Interactions
- Generation of Soot and Species
- Microgravity Combustion
- Droplet and Spray Combustion
- Fire Growth and Suppression
- Diagnostic Developments for Fire and Combustion Systems
- Combustion Synthesis of Materials

Information: W. Gill, STS Certification Environments, P.O. Box 5800, Mail Stop 0853, Sandia National Laboratories, Albuquerque, NM 87185, (505) 845-3193, Fax (505) 844-0078, e-mail: wgill@sandia.gov, Web site: http://www.asme.org/conf/congress99/
Deadline: Abstracts Due by January 29, 1999

NOVEMBER 14-19, 1999

EASTERN ANALYTICAL SYMPOSIUM
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

NOVEMBER 14-19, 1999

ASME INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION
Nashville TN.

Information: P. Pfund, Conference Chair, Babcock and Wilcox, 1562 Beeson Street, Alliance, OH 44601, e-mail: phil.a.pfund@mcdermott.com

NOVEMBER 21-23, 1999

52nd MEETING OF THE AMERICAN PHYSICAL SOCIETY, DIVISION OF FLUID DYNAMICS
New Orleans LA.

Information: M. Gad-el-Hak, Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN 46556, e-mail: mohamed.gad-el-hak.1@nd.edu

NOVEMBER 29-30, 1999

SPQ-99/EUROPE: SPECTROSCOPY IN PROCESS AND QUALITY CONTROL
London, UK.

Information: S. Roberts, Advanstar Communications, Advanstar House, Sealand Road, Chester CH1 4RN, UK, (44) 1244 378 888, Fax: (44) 1244 370 011, e-mail: sroberts@advanstar.com

DECEMBER 7-9, 1999

8th INDIAN SOCIETY FOR MASS SPECTROMETRY SYMPOSIUM
Hyderabad, India.

Information: S.K. Aggarwal, Secretary, ISMAS and Head, Mass Spectrometry Section, Fuel Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India, Fax (91) 22-556-0750, e-mail: skaggr@magnum.barc.ernet.in

JANUARY 6-8, 2000

4th ISHMT/ASME HEAT AND MASS TRANSFER CONFERENCE
Pune Maharashtta, India.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7284, Fax (212) 705-7143, http://www.asme.org

♦ JANUARY 10-13, 2000

38th AIAA AEROSPACE SCIENCES MEETING AND EXHIBIT
Reno NV.

Meeting has Symposia on:

- Aeroacoustics
- Aerodynamic Measurement Technology
- Applied Aerodynamics
- Atmospheric Flight Mechanics
- Microgravity Science and Space Processing
- Plasmadynamics and Lasers
- Propellants and Combustion
- Aerospace Power Systems
- Air-Breathing Propulsion
- Fluid Dynamics
- Intelligent Systems
- Interactive Computer Graphics
- Thermophysics

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JANUARY 10-15, 2000

WINTER CONFERENCE ON PLASMA SPECTROCHEM
Fort Lauderdale FL.

Information: R. Barnes, ICP Info Newsletter, P.O. Box 666, Hadley, MA 01003, e-mail: winterconf@chem.umass.edu

JANUARY 22-28, 2000

PHOTONICS WEST
San Jose CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

♦ MARCH 5-8, 2000

8th INTERNATIONAL CONFERENCE ON NUMERICAL COMBUSTION
Amelia Island FL.

Conference Topics Include:

- Turbulence
- Kinetics
- Detonation
- Flames
- Pollution
- Microgravity
- Ignition
- Applications of Parallel Processing
- Tera-scale Computation of Combustion Applications
- Material Synthesis
- Droplets and Sprays
- Heterogeneous Combustion
- Energetic Materials (Propellants and Explosives)
- Engine and Furnace Combustion
- Fires
- Adaptive Numerical Methods
- Software Engineering for Combustion Applications

Invited Speakers Include:

- Premixed Turbulent Combustion: DNS into Modeling, R. Stewart Cant, University of Cambridge, United Kingdom
- Numerical Modeling of Combustion Control in Ramjets, Sergei Frolov, Semenov Institue of Chemical Physics, Russia
- Aerothermochemistry of Flames, Peter Lindstedt, Imperial College, United Kingdom
- Experimental Measurements of Solid Propellant Flame Structure for Model Validation, Timothy Parr, U.S. Naval Air Warfare Center
- Some New Developments in Pre-Mixed Gaseous Combustion, Gregory I. Sivashinsky, Tel Aviv University, Israel
- The Impact of the Accelerated Strategic Computing Initiative on Numerical Combustion, Charles K. Westbrook Lawrence Livermore National Laboratory

Information: Society for Industrial and Applied Mathematics, 3600 University Science Center, Philadelphia, PA 19104, http://www.siam.org/meetings/

MARCH 6-9, 2000

SAE INTERNATIONAL CONGRESS AND EXPOSITION
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MARCH 13-14, 2000

SPRING MEETING OF THE WESTERN STATES SECTION OF THE COMBUSTION INSTITUTE
Colorado School of Mines, Golden CO.

Information: W.J. Pitz, L-353, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/

MARCH 20-24, 2000

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Minneapolis MN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ MARCH 26-30, 2000

SPRING NATIONAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Atlanta GA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org

MARCH 26-31, 2000

219th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Division of Fuel Science:

- Fuel Science in the Year 2000: Where Do We Stand, Where Do We Go From Here?
  G.P. Huffman, 533 S. Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506-0043, (606) 257-4027, Fax (606) 257-7215 e-mail: cffls@pop.uky.edu
- Advances in F-T Chemistry
  B.H. Davis, Center for Applied Energy Research, University of Kentucky, Lexington, KY 40511, (606) 257-0251, Fax (606) 257-0302, e-mail: davis@alpha.caer.uky.edu
- Molecular Modeling of Solid-Fuel Reactions
  L.R. Radovic, Fuel Science Program, Pennsylvania State University, 217 Academic Projects Building, University Park, PA 16802, (814) 863-0594, Fax (814) 865-3075, e-mail: lrr3@psu.edu

- Applications of X-ray and Gamma Ray Techniques in Fuel Science
  K.A. Carrado, CHM/200, 9700 S. Cass Avenue, Argonne National Laboratory, Argonne, IL 60439-4831, (630) 252-7968, Fax (630) 252-9288, e-mail: kcarrado@anl.gov

Division of Petroleum Chemistry:

- New Chemistry of Fuel Additives
  D. Daly, Fuel Products, Strategic Technology, Lubrizol Co., 29400 Lakeland Blvd., Wickliffe, OH 44092, (440) 943-1200 ext. 4261, Fax (440) 943-9022, e-mail: dtd@lubrizol.com
- CO_2 Conversion and Utilization in Refinery and Chemical Processing
  C. Song, Pennsylvania State University, 209 Academic Projects Building, University Park, PA 16802, (814) 863-4466, Fax (814) 865-3075, e-mail: csong@psu.edu; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com

Division of Physical Chemistry:

- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu; R. Jeanloz, Department of Geology & Geophysics, University of California, Berkeley CA 94720, (510) 642-2639, Fax (510) 643-9980, e-mail: jeanloz@uclink.berkeley.edu
- Atmospheric Chemistry (Harold Johnston Festschrift)
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu

Information: From the Individual Chairpersons or from Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Deadline: 4 Copies of 150-Word Abstract (Original on ACS Abstract Form to Symposium Organizer by August 1, 1999.

MARCH 26-31, 2000

CORROSION/2000
Orlando FL.

Information: NACE Headquarters, Meetings Department, P.O. Box 218340, Houston, TX 77218, (281) 228-6200, Fax (281) 228-6300, http://www.nace.org

♦ APRIL 8-12, 2000

SPRING TECHNICAL CONFERENCE OF THE ASME INTERNAL COMBUSTION ENGINE DIVISION
San Antonio TX.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

♦ APRIL 10-14, 2000

10th INTERNATIONAL IUPAC CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Topics will Include:

- Synthesis, Properties, and Application of High Temperature Materials
- Vaporization, Molecules, and Clusters
- Interface Processes (Corrosion, Oxidation, Diffusion)
- Technical Processes and Devices at High Temperatures
- Thermodynamic and Kinetic Measurements, Modeling and Databases

Information: K. Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnick (IWE 1), 52425 Julich, Germany, (49) 2461 61 3280, Fax (49) 2461 61 3699, e-mail: k.hilpert@fz-juelich.de, http://www.fz-juelich.de/oea/termine.html

APRIL 12-14, 2000

3C STEREO AND HOLOGRAPHIC PIV APPLICATION TO TURBULENCE MEASUREMENTS: EUROMECH COLLOQUIUM 411
Rouen, France.

Information: M. Trinite, CORIA-UMR 6614, Universite et INSA de Rouen, F-76821 Mont Saint Aignan Cedex, France, (33) 2-35-14-65-58, Fax (33) 2-35-70-83-84, e-mail: trinite@coria.fr

APRIL 29-MAY 1, 2000

ANNUAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Long Beach CA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 7-12, 2000

CLEO/QELS 2000
San Francisco CA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, http://www.osa.org/mtg_conf, http://physics.wm.edu/ ~ cooke/dis/dis.html

MAY 8-11, 2000

ASME TURBO EXPO: LAND, SEA AND AIR
Munich, Germany.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072 or (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

MAY 14-19, 2000

197th MEETING OF THE ELECTROCHEMICAL SOCIETY
Toronto, Ontario, Canada.

Topics Include:
- General Session on Corrosion
- Plasma Processing
- 15th International Conference on Chemical Vapor Deposition
- Sensors for Energy Technologies

Information: http://www.electrochem.org/meetings

MAY 16-19, 2000

33rd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Newark DE.

Information: G.L. Trainor, DuPont Pharmaceuticals Co., P.O. Box 80353, Wilmington, DE 19880, (302) 695-3580, Fax (302) 695-8344, e-mail: trainogl@carbon.dmpc.com

MAY 17-19, 2000

32nd CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Covington KY.

Information: R. D'Alonzo, Procter & Gamble, Sharon Woods Technical Center, 11450 Grooms Road, Cincinnati, OH 45242, (513) 626-1977, Fax (513) 626-5145, e-mail: dalonzorp@pg.com

JUNE 4-7, 2000

32nd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Fargo ND.

Information: G.J. McCarthy, North Dakota State University, Department of Chemistry, Ladd Hall 104B, Fargo, ND 58105, (701) 231-7193, Fax (701) 231-8883, e-mail: gmccarth@prarie.nodak.edu

JUNE 8-10, 2000

JOINT 55th NORTHWEST/16th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Idaho Falls ID.

Information: E.G. Meyer, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445.

♦ JUNE 11-15, 2000

SUMMER MEETING OF THE ASME FLUIDS ENGINEERING DIVISION
Boston MA.

Symposia will Include:

- Flows in Manufacturing Processes
- Numerical Developments in CFD
- Non-Invasive Measurements in Multiphase Flow
- Advances in Numerical Modeling of Aerodynamics and Hydrodynamics in Turbomachinery
- Erosion Processes
- Fluid Flow in Microsystems: Measurement, Analysis, and Applications
- Numerical Methods for Multiphase Flows
- Experimental and Numerical Flow Visualization and Laser Anemometry

Forums will be Held on the Following Topics:

- Finite Element Applications in Fluid Dynamics
- Turbulent Flows
- Laminar Flows
- High Speed Jet Flows
- Advances in Fluids Engineering Education
- CFD Applications in Automotive Flows
- Bifurcation, Instability, and Hysteresis in Fluid Flow
- Three-Dimensional Flows
- CFD Applications in Large Facilities
- Open Forum on Multiphase Flows
- Submicron Particle Flows
- Fluid Measurements and Instrumentation
- Fluid Machinery Forum
- Advances in Free Surface and Interface Fluid Dynamics
- Simulation of the Interaction of Transportation Vehicles with the Environment
- Forum on Developments in CFD Code Verification and Validation
- Cavitation and Multiphase Flow Forum

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

JUNE 18-21, 2000

29th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Storrs CT.

Information: G. Epling, University of Connecticut, 215 Glenbrook Road, Storrs, CT 06269, (860) 486-3214, Fax (860) 486-2981, e-mail: epling@nucleus.chem.uconn.edu

♦ JUNE 18-22, 2000

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Salt Lake City UT.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JUNE 18-23, 2000

OPTICS IN COMPUTING
Quebec City, Quebec, Canada.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JUNE 19-20, 2000

CEC/SAE FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION
Le Palais des Congress, Paris, France.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ JULY 1-7, 2000

WORLDWIDE RENEWABLE ENERGY CONGRESS
Brighton UK.

Information: A. Sayrigh, 147 Hilmanton, Lower Earley, Reading RG6 4HN, UK.

JULY 10-13, 2000

10th INTERNATIONAL SYMPOSIUM ON APPLICATIONS OF LASER TECHNIQUES TO FLUID MECHANICS
Lisbon, Portugal.

Information: G. Pereira, Mechanical Engineering Department, Instituto Superior Tecnico, 1049-001 Lisboa, Portugal, Fax (351) 1-849-6156, e-mail: llaser@dem.ist.utl.pt, http://in3.dem.ist.utl.pt/lisboa-laser

JULY 23-28, 2000

ENERGEX 2000: 8th INTERNATIONAL ENERGY FORUM
Las Vegas NV.

Topics will Include:
- Renewable Energies
- Clean Coal Technologies
- Fossil Fuels
- Energy and Economics
- Climatic Change
- International Law
- General Topics
- International Reports
- Nuclear Energy
- Architecture

Information: P. Catania, Faculty of Engineering, University of Regina, Regina, SK S4S 0A2, Canada, (306) 585-4363, Fax (306) 585-4855, e-mail: peter.catania@uregina.ca, http://www2.regina.ism.ca/ief/index/htm or http://www.energysource.com/ief/updates/

♦ JULY 24-28, 2000

35th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

JULY 30-AUGUST 4, 2000

SPIE ANNUAL MEETING
San Diego CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 30-AUGUST 4, 2000

28th INTERNATIONAL SYMPOSIUM ON COMBUSTION
Edinburgh, Scotland.

Information: S.S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh, PA 15212, (412) 687-1366, Fax (412) 687-0340, e-mail: combust@telerama.lm.com

AUGUST 1-5, 2000

35th IECEC INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

AUGUST 20-24, 2000

220th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Washington DC.

Division of Fuel Chemistry:

- 1990 Clean Air Act Amendments: A 10-Year Assessment
  J.J. Helble, University of Connecticut, Department of Chemical Engineering, U-222, Storrs, CT 06269, (860) 486-4602, Fax (860) 486-2959, e-mail: helble@eng2.uconn.edu
- Inorganics in Fossil Fuels, Waste Materials, and Biomass: Characterization, Combustion Behavior, and Environmental Issues
  C.L. Senior, Physical Sciences, Inc., 20 New England Business Center, Andover, MA 01810, (978) 689-0003, Fax (978) 689-3232, e-mail: senior@psicorp.com
- Waste Material Recycling for Energy and Other Applications
  S.V. Pisupati, Fuel Science Program, Pennsylvania State University, 404 Academic Projects Building, University Park, PA 16802, (814) 865-0874, Fax (814) 863-8892, e-mail: sxp17@psu.edu
- Fossil Fuels and Global Climate/CO_2 Abatement
  R. Warzinski, USDOE/FETC, Box 10940, Building 83-324, Pittsburgh, PA 15236, (412) 892-5863, e-mail: warzinsk@fetc.doe.gov

Division of Petroleum Chemistry:

- Emission Control in Petroleum Processing
  P. O'Connor, U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu
- Structure of Jet Fuels VI
  W.E. Harrison, Department of the Air Force, WL/POSF, Building 490, Area B, 1790 Loop Road N., Wright-Patterson AFB, OH 45433, (937) 255-6601, Fax (937) 255-1125, e-mail: harriswe@wl.pafb.af.mil

Information: From the Individual Chairpersons or from the Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ AUGUST 20-22, 2000

34th ASME NATIONAL HEAT TRANSFER CONFERENCE
Pittsburgh PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7795, Fax (212) 705-7143, http://www.asme.org

AUGUST 22-25, 2000

9th INTERNATIONAL (MILLENNIUM) SYMPOSIUM ON FLOW VISUALIZATION
Edinburgh, Scotland.

Information: I. Grant, Heriot-Watt University, Edinburgh, Scotland, EH10 5PJ, UK, (44) 1314478800, Fax (44) 1314478660, e-mail: 9misfv@ode-web.demon.co.uk, Web Site: http://www.ode-web.demon.co.uk/9misfv
Deadline: Abstract Template should be Downloaded from the Web. 4 Pages or Less to be Submitted by December 12, 1999. Final Manuscripts Due May 15, 2000.

♦ SEPTEMBER 10-13, 2000

3rd EUROPEAN THERMAL SCIENCES CONFERENCE
Heidelberg, Germany.

Information: E. Hahne, Institut fur Thermodynamik und Warmetechnik, Pfaffenwaldring 6, 70550 Stuttgart, Germany, 49 (0) 711-685-3536, Fax 49 (0) 711-685-3503, e-mail: pm@itw.uni-stuttgart.de

SEPTEMBER 10-15, 2000

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

SEPTEMBER 19-21, 2000

THE HYDROGEN ENERGY FORUM 2000
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

SEPTEMBER 22-30, 2000

27th ANNUAL CONFERENCE OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

♦ SEPTEMBER 23-26, 2000

ASME FALL TECHNICAL CONFERENCE OF THE INTERNAL COMBUSTION ENGINE DIVISION
Peoria IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

♦ OCTOBER 8-11, 2000

GASIFICATION TECHNOLOGIES CONFERENCE
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

OCTOBER 16-19, 2000

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

♦ NOVEMBER 5-10, 2000

ASME INTERNATIONAL MECHANICAL ENGINEERING CONFERENCE AND EXHIBITION
Orlando FL.

Symposia will Include:

- Symposium on Multiphase Flow in Biomedical Applications and Processes
- Dispersed Flows in Combustion, Incineration, and Propulsion Systems
- Application of Microfabrication to Fluid Mechanics

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 13-18, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

DECEMBER 6-8, 2000

JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

DECEMBER 14-19, 2000

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

MARCH 12-16, 2001

ANNUAL MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Seattle WA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 6-11, 2001

CLEO/QELS 2001
Baltimore MD.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

MAY 20-25, 2001

FLUIDIZATION X
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

♦ JUNE 24-28, 2001

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Orlando FL.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JULY 9-11, 2001

COMBUSTION CHEMISTRY: ELEMENTARY REACTIONS TO MACROSCOPIC PROCESSES: FARADAY DISCUSSION NUMBER 119
Leeds, UK.

Joint Meeting with the British Section of the Combustion Institute.
Information: M. Pilling, School of Chemistry, University of Leeds, Leeds UK, e-mail: m.j.pilling@chem.leeds.ac.uk, http://www.chem.leeds.ac.uk

AUGUST 20-24, 2001

13th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, (358) 2-265-4295, Fax (358) 2-265-4706, e-mail: icofts@abo.fi, http://www.abo.fi/icofts

OCTOBER 5-12, 2001

28th ANNUAL MEETING OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Detroit MI.

Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

CURRENT BIBLIOGRAPHY RELEVANT TO FUNDAMENTAL COMBUSTION

March 1999

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

1. FUELS/SYNFUELS - GENERAL

80058. Vaughan, R.D., ed., "*2020 Vision. The Engineering Challenges of Energy: The Full Report and Recommendations of the Engineering Institutions,*" Special Issue *Proc. Inst. Mech. Eng. A. J. Power Energy* 212, 389-483 (1998).

Energy
Fuel Supply
Conversions
Usage,Trends
Reviews

(80110) (80111) Chemical Loop Combustion, MO+Fuel Produces M, then M+O_2 Provides Energy

Fuel Energy Cycle

80059 Jones, J.C., "Reid Vapor Pressure as a Route to Calculating the Flash Points of Petroleum Fractions," *J. Fire Sci.* 16, 222-229 (1998).

Petroleum Fractions
Flash Points
Vapor Pressure
Estimation Method

80060. Pantskhava, E.S., V.A. Pozharnov, M.I. Maiorov and I.I. Shkola, "Biogas Technologies and the Solution to Problems of Biomass and the Greenhouse Effect in Russia," *Thermal Eng., Russia* 46, 115-125 (1999).

Biomass Fuels
Economic Feasibility
Zero CO_2 Solution

80061. Karaosmanoglu, F., "Vegetable Oil Fuels: A Review," *Energy Sources* 21, 221-231 (1999).

Vegetable Oil Fuels
Review

2. LIQUEFACTION/GASIFICATION

80062. Deutschmann, O., and L.D. Schmidt, "Modeling the Partial Oxidation of Methane in a Short Contact Time Reactor," *AIChE J.* 44, 2465-2477 (1998).

Catalytic Partial Oxidation
CH_4/O_2/Rh,Pt
CO,H_2
Conversions
Model

80063. Hu, Y.H., and E. Ruckenstein, "Isotopic Gas Chromatography Mass Spectral Study of the Mechanism of Methane Partial Oxidation to Synthesis Gas," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10568-10571 (1998).

Catalytic Partial Oxidation
$CH_4/CD_4/O_2$
Mechanism

80064. Larkin, D.W., T.A. Caldwell, L.L. Lobban and R.G. Mallinson, "Oxygen Pathways and Carbon Dioxide Utilization in Methane Partial Oxidation in Ambient Temperature Electric Discharges," *Energy Fuels* 12, 740-744 (1998).

Partial Oxidation
$CH_4/O_2/(CO_2)$
CH_3OH,CH_2O
$HCOOH,HCOOCH_3$
Product Yields
CO,CO_2 Effects

80065. Zhou, L.M., B. Xue, U. Kogelschatz and B. Eliasson, "Nonequilibrium Plasma Reforming of Greenhouse Gases to Synthesis Gas," *Energy Fuels* 12, 1191-1199 (1998).

Fuel Reforming
CH_4/CO_2
Discharge
CO/H_2
Synfuel Yields

80066. Sekine, Y., T. Nishimura and K. Fujimoto, "Oxidative Coupling of Methane in the Gas Phase: Simulation and Reaction Mechanism," *Energy Fuels* 12, 828-829 (1998).

Fuel Conversion
$CH_4/O_2/N_2$
Flow Reactor
C_2,C_3,CO,CO_2
Product Yields

80067. Gaudernack, B., and S. Lynum, "Hydrogen from Natural Gas without Release of CO_2 to the Atmosphere," *Int. J. Hydrogen Energy* 23, 1087-1093 (1998).

Fuel Conversion
CH_4 to H_2
Carbon Sequestration Methods

(80530) Thermal Cracking, C_2H_4, C_3H_6 Product Yields

C_3H_8/O_2/Steam

80068. Sharma, R.K., J.W. Zondlo and D.B. Dadyburjor, "A Kinetic Scheme for Catalytic Coliquefaction of Coal and Waste Tire," *Energy Fuels* 12, 589-597 (1998).

Catalytic Liquefaction
Coal/Tires
Ferric Sulfide Catalyst
Primary Products
Mechanisms

80069. Sharma, R.K., D. Tian, J.W. Zondlo and D.B. Dadyburjor, "Two-Stage Catalytic Coliquefaction of Coal and Waste Tire," *Energy Fuels* 12, 1245-1255 (1998).

Catalytic Liquefaction
Coal/Tires
Two Stage Process
Oil Yields

3. BURNERS

(See also Section 21 for Burner Emissions and Incinerator Performance)

80070.	Gupta, A.K., M.J. Lewis and S. Qi, "Effect of Swirl on Combustion Characteristics in Premixed Flames," Presented Originally as Paper 97-GT-276 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 488-494 (1998).	Swirl Burner Double Concentric Premixed CH_4/Air T,Thermocouples Flame Structure
80071.	Fu, X., R. Viskanta and J.P. Gore, "Combustion and Heat Transfer Interaction in a Pore-Scale Refractory Tube Burner," *J. Thermophys. Heat Transfer* 12, 164-171 (1998).	Porous Ceramic Radiant Burner 2-D Model Heat Transfer
(80112)	CH_4/Air Incineration of VOCs	Foam Ceramic Burner
(80014)	Gas Turbine Applications, Low NO_x Emissions	Catalytic Combustor
80072.	Bannister, R.L., R.A. Newby and W.C. Yang, "Development of a Hydrogen Fueled Combustion Turbine Cycle for Power Generation," Presented Originally as Paper 97-GT-14 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 276-283 (1998).	Gas Turbine H_2/O_2 Development
80073.	Wikstrom, E., P. Andersson and S. Marklund, "Design of a Laboratory Scale Fluidized Bed Reactor," *Rev. Sci. Instrum.* 69, 1850-1859 (1998).	FB Reactor Laboratory Scale Design

4. COAL, PARTICLE COMBUSTION/PYROLYSIS

(80330)	NO_x Emissions, US Assessments	Coal Fired Electric Utilities
(80329)	PAH Emissions, 5 Power Plant Data	Coal Combustion
(80348)	Soot Formation, Semiempirical Model, Transport/Radiative Properties	Pulverized Coal Combustion
(80335)	NO_x Formation, Reactor Air Staging, Nitrogen Fate Measurements	Coal Combustion
80074.	Joutsenoja, T., J. Saastamoinen, M. Aho and R. Hernberg, "Effects of Pressure and Oxygen Concentration on the Combustion of Different Coals," *Energy Fuels* 13, 130-145 (1999).	Coal Particle Combustion Pressure,O_2 Coal Type Effects
80075.	Medek, J., and Z. Weishauptova, "Effect of Coal Interaction with Oxygen on Its Ignition Temperature," *Energy Fuels* 13, 77-81 (1999).	Coal Self-ignition Dry/Moist O_2 Interactions Measurements
(80859)	Vapor Pressures, Measurements	Coal Tars

80076.	Monazam, E.R., L.J. Shadle and A. Shamsi, "Spontaneous Combustion of Char Stockpiles," *Energy Fuels* 12, 1305-1312 (1998).	Char Stockpiles Spontaneous Combustion Model
80077.	Stanczyk, K., "Nitrogen Oxide Evolution from Nitrogen-Containing Model Chars Combustion," *Energy Fuels* 13, 82-87 (1999).	Char Combustion NO_x Formation Char 'N' Structural Dependences
(80068) (80069)	Processes, Oil Yields, Mechanisms	Coal/Tire Liquefaction
80078.	Cunliffe, A.M., and P.T. Williams, "Properties of Chars and Activated Carbons Derived from the Pyrolysis of Used Tires," *Environ. Technol.* 19, 1177-1190 (1998).	Tire Pyrolysis Char Activated Carbons Yields
80079.	Williams, P.T., and J.M. Nazzal, "Polycyclic Aromatic Compounds in Shale Oils: Influence of Process Conditions," *Environ. Technol.* 19, 775-787 (1998).	Oil Shales Pyrolysis Product Oil PAH Content Steam Effects
80080.	Egolfopoulos, F.N., and C.S. Campbell, "Dynamics and Structure of Dusty Reacting Flows: Inert Particles in Strained, Laminar, Premixed Flames," *Combust. Flame* 117, 206-226 (1999).	Inert Particles/ H_2/Air Interactions Modeling Size,Gravity Effects
(80138)	Ignition, Hot Environments, Particle Sizes, Layer Depths, Dependences	Dust Layers
80081.	Goroshin, S., J.H.S. Lee and Yu. Shoshin, "Effect of the Discrete Nature of Heat Sources on Flame Propagation in Particulate Suspensions," *Int. Symp. Combust.* 27, 743-749 (1998).	Dust Flames Burning Velocities Propagation Heat Transfer Models

5. SPRAY COMBUSTION

(See also Section 23 for Droplet Characterization)

80082.	Miller, R.S., K. Harstad and J. Bellan, "Evaluation of Equilibrium and Nonequilibrium Evaporation Models for Many-Droplet Gas-Liquid Flow Simulations," *Int. J. Multiphase Flow* 24, 1025-1055 (1998).	Many Droplet Vaporization Flow Simulation Model

80083.	Kohnen, G., and M. Sommerfeld, "Numerical Calculations of Evaporating Turbulent Sprays," *Chem. Technik* 50, 225-234 (1998).	Sprays Evaporation Turbulent Hollow Cone/ Heated Air PDA Modeling
80084.	Santangelo, P.J., and I.M. Kennedy, "Droplet Lasing Spectroscopy Applied to Droplet Stream Flames," *Combust. Flame* 117, 413-421 (1999).	Droplet Streams Reacting/ Nonreacting Vaporization Rates Laser Monitoring Method Sizes
80085.	Sommerfeld, M., and H.-H. Qiu, "Experimental Studies of Spray Evaporation in Turbulent Flow," *Int. J. Heat Fluid Flow* 19, 10-22 (1998).	Spray Evaporation Heated Turbulent Air Stream *i*-C_3H_7OH PDA Sizes,Velocities
80086.	Daif, A., M. Bouaziz and M. Grisenti, "Vaporization of Binary Fuel Mixture Droplets in a Thermal Wind Tunnel," *J. Thermophys. Heat Transfer* 12, 107-113 (1998).	Droplets Binary Fuels Vaporization $C_7H_{16}/C_{10}H_{22}$ Measurements
(80214)	Unconfined Clouds, Detonations, Initiation Energies	Gasoline Spray
80087.	Char, J.M., W.J. Liou, J.H. Yeh and C.L. Chiu, "Ignition and Combustion Study of JP-8 Fuel in a Supersonic Flowfield," *Shock Waves* 6, 259-266 (1996).	Supersonic Flows JP-8 Droplet Combustion Ignition Delays Modeling
80088.	Wichman, I.S., and M. Yang, "Double-Spray Counterflow Diffusion Flame Model," *Combust. Theory Modeling* 2, 373-398 (1998).	Double Spray Counterflow Flame Model
80089.	Seiser, R., L. Truett, D. Trees and K. Seshadri, "Structure and Extinction of Nonpremixed *n*-Heptane Flames," *Int. Symp. Combust.* 27, 649-657 (1998).	Counterflow Vapor Flame *n*-C_7H_{16}/Air Microprobe/GC Species Profiles Liquid Pool Flame Comparison

80090. Huang, L.-W., and C.-H. Chen, "Numerical Analysis of a Burning Droplet with Internal Circulation in a Gravitational Environment," *Numer. Heat Transfer A. Applications* 34, 43-60 (1998).

Droplet Combustion Internal Circulation Effects Numerical Analysis

80091. Kim, Y.M., S.J. Kim, Z.J. Chen and C.P. Chen, "Numerical Simulation of Combustion Wave Propagation in an Air/Fuel Spray Mixture with Temperature Nonuniformity," *Numer. Heat Transfer A. Applications* 34, 23-41 (1998).

Fuel Spray Propagation Detonation Wave Numerical Modeling

80092. Golovanevsky, B., Y. Levy, J.B. Greenberg and M. Matalon, "On the Oscillatory Behavior of Laminar Spray Diffusion Flames: Experiment and Theory," *Combust. Flame* 117, 373-383 (1999).

Spray Diffusion Oscillatory Combustion

80093. Avedisian, C.T., B.J. Callahan and G.S. Jackson, "Soot Shell Structures of Fuel Droplet Flames in Microgravity," *J. Heat Transfer, Trans ASME* 120, 544 (1998).

Fuel Droplet Microgravity Combustion Soot Shell Structures n-C_7H_{16} ,n-C_9H_{20} Visualization

6. METALS/PROPELLANTS/POLYMER COMBUSTION

80094. Frankel, M., V. Roytburd and G. Sivashinsky, "Complex Dynamics Generated by a Sharp Interface Model of Self-Propagating High Temperature Synthesis," *Combust. Theory Modeling* 2, 479-496 (1998).

Solid Phase Combustion Propagation Numerical Modeling

80095. Myagkov, V.G., L.E. Bykova and V.A. Seredkin, "Oscillations of the Front of Self-Propagating High Temperature Synthesis in Two-Layer Thin Films," *Dokl. Phys.* 43, 768-770 (1998).

Solid Phase Combustion 2-Layer Thin Film Propagation Oscillations

(80136) Fire Ignition, Solid/Gas Phase Flame, Mechanisms

Solid Phase Combustion

80096. Mercer, G.N., R.O. Weber and H.S. Sidhu, "An Oscillatory Route to Extinction for Solid Fuel Combustion Waves Due to Heat Losses," *Proc. Roy. Soc. Lond. A* 454, 2015-2022 (1998).

Solid Fuel Combustion Oscillations Heat Loss Extinction Mechanism

80097. Bucher, P., R.A. Yetter, F.L. Dryer, E.P. Vicenzi, T.P. Parr and D.M. Hanson-Parr, "Condensed-Phase Species Distributions about Al Particles Reacting in Various Oxidizers," *Combust. Flame* 117, 351-361 (1999).

Al Particle
Combustion
Condensed Phase
Product
Distributions

80098. Foelsche, R.O., R.L. Burton and H. Krier, "Boron Particle Ignition and Combustion at 30-150 atm," *Combust. Flame* 117, 32-58 (1999).

Boron Particles
Ignition
Combustion
$H_2/O_2/N_2$
Size Effects

80099. Zhou, W., R.A. Yetter, F.L. Dryer, H. Rabitz, R.C. Brown and C.E. Kolb, "Multiphase Model for Ignition and Combustion of Boron Particles," *Combust. Flame* 117, 227-243 (1999).

Boron Particles
Combustion
Multiphase Model
F Effects
Species Profiles
Kinetic Model

80100. Park, H.K., Y.S. Han, D.K. Kim and C.H. Kim, "Synthesis of $LaCrO_3$ Powders by Microwave Induced Combustion of Metal Nitrate-Urea Mixture Solution," *J. Mater. Sci. Lett.* 17, 785-787 (1998).

$LaCrO_3$
Powder Synthesis
Metal Nitrates/
Urea
Induced Combustion

80101. Akiyama, T., H. Isogai and J.-i. Yagi, "Mathematical Model of Combustion Synthesis," *AIChE J.* 44, 695-700 (1998).

Mg/Ni
Solid Phase
Partial Melting
Combustion
Modeling

80102. Chandramouli, V., S. Anthonysamy and P.R. Vasudeva Rao, "Combustion Synthesis of Thoria: A Feasibility Study," *J. Nuclear Materials* 265, 255-261 (1999).

ThO_2 Powder
Synthesis
Solid Phase
Combustion
$Th(NO_3)_4/CO(NH_2)_2$
Citric Acid

80103. Ward, M.J., S.F. Son and M.Q. Brewster, "Role of Gas and Condensed-Phase Kinetics in Burning Rate Control of Energetic Solids," *Combust. Theory Modeling* 2, 293-312 (1998).

Energetic Materials
Combustion Rates
Gas Phase
Role
Modeling

80104. Lee, Y.J., C.-J. Tang and T.A. Litzinger, "A Triple Quadrupole Mass Spectrometer System for Studies of Gas Phase Combustion Chemistry of Energetic Materials," *Measurement Sci. Technol.* 9, 1576-1586 (1998).

Energetic Materials
Dissociation
Product Analysis
Mass Spectral
Method

80105. Strunin, V.A., A.P. D'Yakov and G.B. Manelis, "Combustion of Ammonium Dinitramide," *Combust. Flame* 117, 429-434 (1999).

ADM
$NH_4N(NO_2)_2$
Burning Rate
Combustion Products

80106. Tang, C.-J., Y.J. Lee and T.A. Litzinger, "Simultaneous Temperature and Species Measurements of the Glycidyl Azide Polymer (GAP) Propellant During Laser Induced Decomposition," *Combust. Flame* 117, 244-256 (1999).

GAP
Laser Induced Dissociation
T,Species
Microprobe Mass Analysis

80107. Tang, C.-J., Y.J. Lee, G. Kudva and T.A. Litzinger, "A Study of the Gas Phase Chemical Structure During CO_2 Laser Assisted Combustion of HMX," *Combust. Flame* 117, 170-188 (1999).

HMX
Laser Assisted Combustion
Major Species Profiles

80108. Kellogg, D.S., B.E. Waymack, D.D. McRae, P. Chen and R.W. Dwyer, "The Initiation of Smoldering Combustion in Cellulosic Fabrics," *J. Fire Sci.* 16, 90-104 (1998).

Cellulosic Fabrics
Smoldering Initiation
Combustion
Na,K Effects

80109. Williams, P.T., and E.A. Williams, "Interaction of Plastics in Mixed-Plastics Pyrolysis," *Energy Fuels* 13, 188-196 (1999).

Mixed Plastics
Pyrolysis
Gas/Liquid Products

7. CATALYTIC COMBUSTION

(See also Section 2 for Catalytic Liquefaction and Gasification)

80110. Ishida, M., H. Jin and T. Okamoto, "Kinetic Behavior of Solid Particle in Chemical-Looping Combustion: Suppressing Carbon Deposition in Reduction," *Energy Fuels* 12, 223-229 (1998).

Chemical Loop Combustion
MO+Fuel/M
$M+O_2$/Energy
Carbon Formation Suppression

80111. Jin, H., T. Okamoto and M. Ishida, "Development of a Novel Chemical-Looping Combustion: Synthesis of a Looping Material with a Double Metal Oxide of CoO-NiO," *Energy Fuels* 12, 1272-1277 (1998).

Chemical Loop Combustion
MO+Fuel/M
$M+O_2$/Energy
CoO/NiO Catalyst Performance

(80071) Heat Transfer, 2-D Model

Porous Ceramic Radiant Burner

80112. Goralski Jr, C.T., L.D. Schmidt and W.L. Brown, "Catalytic Incineration of Volatile Organic Compounds (VOC) Containing Air Streams at Very Short Contact Times," *AIChE J.* 44, 1880-1888 (1998).

Catalytic Incineration
VOCs
Foam Ceramic Burner
CH_4/Air

80113. Stolle, S., U. Hatje, H. Forster and R. Salzer, "Zeolite Catalyzed Low Temperature Gas Phase Combustion of Environmentally Harmful Arenes," *Chem. Technik* 50, 287-292 (1998).

Zeolite
Catalytic Combustion
C_6H_5Cl/Air
Waste Disposal

80114. Fujii, T., Y. Ozawa, S. Kikumoto, M. Sato, Y. Yuasa and H. Inoue, "High Pressure Test Results of a Catalytic Combustor for Gas Turbine," Presented Originally as Paper 96-GT-382 at the *41st International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Birmingham UK, June 1996, *J. Eng. Gas Turbines, Trans. ASME* 120, 509-513 (1998).

Catalytic Combustor
Gas Turbine Application
Low NO_x

80115. Widjaja, H., K. Sekizawa and K. Eguchi, "Catalytic Combustion of Methane over Pd Supported on Metal Oxides," *Chem. Lett. Jpn.* 481-482 (1998).

Catalytic Combustion
CH_4/O_2/Pd
Low Temperatures

80116. Zhao, Z., A. Obuchi, J. Uchisawa, A. Ogata and S. Kushiyama, "Autonomous Improvement in the Catalytic Activity of KVO_3/SiC for Soot Oxidation under Practical Gaseous Conditions," *Chem. Lett. Jpn.* 367-368 (1998).

Catalytic Combustion
Soot Oxidation

80117. Imada, Y., N. Kakuta, A. Ueno and K. Yoshida, "Effects of Cl Ions upon Combustion of Particulate on TiO_2 Supported CuO Catalysts," *Chem. Lett. Jpn.* 363-364 (1998).

CuO/TiO Catalyst
Soot Oxidation
Cl^- Effects

80118. Park, Y.K., P.-A. Bui and D.G. Vlachos, "Operation Regimes in Catalytic Combustion: H_2/Air Mixtures Near Pt," *AIChE J.* 44, 2035-2043 (1998).

Catalytic Combustion
H_2/Air/Pt
Flammability Limits

80119. Schaak, A., S. Shaikhutdinov and R. Imbihl, "H/D Isotope Effects in Chemical Wave Propagation on Surfaces: The O_2+H_2 and $NO+H_2$ Reactions on Rh(110) and Rh(111)," *Surface Sci.* 421, 191-203 (1999).

Catalytic
H_2/O_2/Rh
NO/H_2/Rh
Isotope Effects
Propagation

8. MHD

9. TEMPERATURES

(See Section 32 for 2-D Temperature Mapping Measurements)

80120. Young, K.J., S.N. Ireland, M.C. Melendez-Cervates and R. Stones, "On the Systematic Error Associated with the Measurement of Temperature using Acoustic Pyrometry in Combustion Products of Unknown Mixture," *Measurement Sci. Technol.* 9, 1-5 (1998).

Temperatures
Acoustic Pyrometry
Combustion
Application
Errors

80121. Ewan, B.C.R., "A Study of Two Optical Fiber Probe Designs for Use in High Temperature Combustion Gases," *Measurement Sci. Technol.* 9, 1330-1335 (1998).

Temperatures
Pyrometry
Optical Fibers
Emission Method
1650-1900 °C

80122. Pitts, W.M., K.C. Smyth and D.A. Everest, "Effects of Finite Time Response and Soot Deposition on Thin Filament Pyrometry Measurements in Time-Varying Diffusion Flames," *Int. Symp. Combust.* 27, 563-569 (1998).

Temperatures
Pyrometry
Thin Filaments
Time Response
Soot Deposition
Errors

(80474) T_{exc}, T_{rot} Plasma Characterization, Microwave Discharge

Fe*
N_2^+(B-X),(0,0)

80123. Scott, C.D., H.E. Blackwell, S. Arepalli and M.A. Akundi, "Techniques for Estimating Rotational and Vibrational Temperature in Nitrogen Arcjet Flow," Presented Originally as AIAA Paper 97-2521 at the *32nd AIAA Thermophysics Conference*, Held in Atlanta GA, June 1997, *J. Thermophys. Heat Transfer* 12, 457-464 (1998).

Temperatures
Vibrational
Rotational
N_2,N_2^+
Arcjet
Shock Layer

80124. Blackwell, H.E., C.D. Scott and S. Arepalli, "Measured Shock Layer Vibrational Populations and Temperatures in Arcjet Nitrogen Flow," Presented Originally as AIAA Paper 97-2522 at the *32nd AIAA Thermophysics Conference*, Held in Atlanta GA, June 1997, *J. Thermophys. Heat Transfer* 12, 465-472 (1998).

Temperatures
Vibrational
Rotational
N_2,N_2^+
Arcjet
Shock Layer

80125. Koulidiati, J., A. Czernichowski, J.J. Beulens and D.C. Schram, "Diagnostics of a Hydrocarbon Plasma Jet Using the ($A^2\Delta$-$X^2\Pi$) System of CH," *Acta Phys. Pol. A* 94, 3-12 (1998).

Temperatures
Rotational
Vibrational
CH(A-X)
Plasma Jet

80126. Rousseau, A., E. Teboul and P. Leprince, "Time Resolved Temperature Measurements in a H_2 High Power Pulsed Discharge," *J. de Phys. IV. Colloque* 8(7), 287-295 (1998).

Temperatures
Rotational
Translational
H_2
Pulsed
Microwave Discharge

80127. Ke, C.-B., and K.-C. Lin, "Spatially Resolved Temperature Determination of an Air/Acetylene Flame Using the Two-Step Laser Enhanced Ionization Technique," *Appl. Spectrosc.* 52, 187-194 (1998).

Temperatures
2-Step
Laser Enhanced
Ionization
Al,Ga
C_2H_2/Air Flame

(80280) Indium 2-Line Fluorescence Method, I.C. Engines

2-D Temperatures

80128. Buckner, S.W., R.A. Forlines and J.R. Gord, "Liquid Phase Thermometry Based on Fluorescence Lifetimes of Intramolecular Excimers," *Appl. Spectrosc.* 53, 115-119 (1999).

Temperatures
Jet-A Fuel
$C_{12}H_{26}$ Liquids
Excimer LIF
Method

80129. Palma, P.C., T.J. McIntyre and A.F.P. Houwing, "PLIF Thermometry in Shock Tunnel Flows Using a Raman Shifted Tunable Excimer Laser," *Shock Waves* 8, 275-284 (1998).

Temperatures
PLIF,NO
Shock Tunnel
Measurements

80130. Boyce, R.R., D.R.N. Pulford, A.F.P. Houwing and C. Mundt, "Rotational and Vibrational Temperature Measurements Using CARS in a Hypervelocity Shock Layer Flow and Comparisons with CFD Calculations," *Shock Waves* 6, 41-51 (1996).

Temperatures
CARS,N_2
Rotational
Vibrational
Hypervelocity
Flows

10. IGNITION

80131. Amano, T., and F.L. Dryer, "Effect of Dimethyl Ether, NO_x , and Ethane on CH_4 Oxidation: High Pressure, Intermediate Temperature Experiments and Modeling," *Int. Symp. Combust.* 27, 397-404 (1998).

Auto-ignition
CH_4/O_2
Additive
$(CH_3)_2O,C_2H_6$
NO_x
Effects
Kinetic Modeling

80132. Ribaucour, M., R. Minetti and L.R. Sochet, "Auto-ignition of *n*-Pentane and 1-Pentene: Experimental Data and Kinetic Modeling," *Int. Symp. Combust.* 27, 345-351 (1998).

Auto-ignition
C_5H_{10} ,C_5H_{12}
Kinetic Model
Data Comparisons

80133. Westbrook, C.K., H.J. Curran, W.J. Pitz, J.F. Griffiths, C. Mohamed and S.K. Wo, "The Effects of Pressure, Temperature and Concentration on the Reactivity of Alkanes: Experiments and Modeling in a Rapid Compression Machine," *Int. Symp. Combust.* 27, 371-378 (1998).

Auto-ignition
n-$C_5H_{12}/O_2/Ar$
Product Species
Stirred Reactor
Kinetic Modeling

80134. Curran, H.J., W.J. Pitz, C.K. Westbrook, C.V. Callahan and F.L. Dryer, "Oxidation of Automotive Primary Reference Fuels at Elevated Pressures," *Int. Symp. Combust.* 27, 379-387 (1998).

Auto-ignition
n-C_7H_{16}, i-C_8H_{18}
High Pressure
Flow Reactor
Products
Kinetic Modeling

80135. Tosaka, Y., H. Shoji and A. Saima, "A Study of the Influence of Intermediate Combustion Products on Knocking," *JSAE Review* 16, 233-238 (1995).

Auto-ignition
n-C_7H_{16}, i-C_8H_{18}
I.C. Engine
End,Center Zones
CH, C_2, OH
Spectral Absorption
Behaviors

(80075) Dry/Moist O_2 Interactions, Measurements

Coal
Self-ignition

(80076) Stockpiles, Combustion, Model

Char
Self-ignition

(80087) JP-8 Droplet Combustion, Supersonic Flows, Modeling

Ignition Delays

80136. Atreya, A., "Ignition of Fires," *Phil. Trans. Roy. Soc. Lond. A* 356, 2787-2813 (1998).

Fire Ignition
Solid Phase
Initiated
Gas Phase Flame
Mechanisms

80137. Forbes, L.K., and B.F. Gray, "Burning Down the House: The Time to Ignition of an Irradiated Solid," *Proc. Roy. Soc. Lond. A* 454, 2667-2688 (1998).

Ignition
Wood
Thermal Radiation
Initiation
Modeling

80138. Sweis, F.K., "The Effect of Admixed Material on the Ignition Temperature of Dust Layers in Hot Environments," *J. Hazardous Mat.* A63, 25-35 (1998).

Ignition
Dust Layers
Particle Sizes
Layer Depths
Dependences

(80212) Detonations, Instabilities, Theory

Re-ignition

(80098) Ignition in an $H_2/O_2/N_2$ Flame, Combustion, Size Effects

Boron Particles

(80834) Combustion Reactions, ΔH_f(B/H/C/O/F) Molecules, $\Delta H_{Reaction}$, Calculations

Boron Ignition

80139. Slutsky, V.G., S.A. Tsyganov and E.S. Severin, "The Mechanism of High Temperature Oxidation of Carborane $C_2B_4H_6$ by Water Vapor," *Int. Symp. Combust.* 27, 405-411 (1998).

Ignition Delays
$B_4C_2H_6/H_2O$
Combustion Products Mechanisms

(80522) Shock Ignition, Elevated Pressures, Kinetic Modeling

CH_4/O_2

80140. Egolfopoulos, F.N., and P.E. Dimotakis, "Nonpremixed Hydrocarbon Ignition at High Strain Raates," *Int. Symp. Combust.* 27, 641-648 (1998).

Ignition
CH_4/C_2H_4
High Strain Rates
H_2,F_2 Effects
Transport/Kinetic Modeling

80141. Dagaut, P., C. Daly, J.M. Simmie and M. Cathonnet, "The Oxidation and Ignition of Dimethylether from Low to High Temperature (500-1600 K): Experiments and Kinetic Modeling," *Int. Symp. Combust.* 27, 361-369 (1998).

Ignition
$(CH_3)_2O/O_2$
Stirred Reactor
Species Profiles
Kinetic Modeling

(80287) I.C. Engine, Gasoline Additives, Ignition Effects, Hydrocarbon, CO, NO_x Emissions

Furan,*p*-Cresol

(80170) Counterflow H_2,N_2/Air Diffusion Flames, Strained by an Impinging Microjet, Extinction, 2-D Temperature Mapping

Re-ignition

80142. Sanchez, A.L., I. Iglesias and A. Linan, "As Asymptotic Analysis of Chain-Branching Ignition in the Laminar Wake of a Splitter Plate Separating Streams of Hydrogen and Oxygen," *Combust. Theory Modeling* 2, 259-271 (1998).

Ignition
H_2/O_2
Split Flows
Asymptotic Analysis
H Atom Profile

80143. Aghalayam, P., P.-A. Bui and D.G. Vlachos, "The Role of Radical Wall Quenching in Flame Stability and Wall Heat Flux: Hydrogen/Air Mixtures," *Combust. Theory Modeling* 2, 515-530 (1998).

Ignition
H_2/Air
Wall Quenching Role
Modeling

11. COMBUSTION THEORY/PROPAGATION/STABILIZATION

80144. Wang, S.-H., "Rigorous Analysis and Estimates of S-Shaped Bifurcation Curves in a Combustion Problem with General Arrhenius Reaction Rate Laws," *Proc. Roy. Soc. Lond. A* 454, 1031-1048 (1998).

Combustion Theory
Arrhenius Kinetics
Bifurcation Analysis

(80213) Propagation, Deflagration/Detonation Transitions

Porous Medium

80145.	Baum, H.R., and W.E. Mell, "A Radiative Transport Model for Large-Eddy Fire Simulations," *Combust. Theory Modeling* 2, 405-422 (1998).	Fire Simulation 3-D Buoyant Radiative Modeling
80146.	Grant, G.B., S.F. Jagger and C.J. Lea, "Fires in Tunnels," *Phil. Trans. Roy. Soc. Lond. A* 356, 2873-2906 (1998).	Tunnel Fires Ventilation Hot Smoke Layers Model Inadequacies
80147.	Cox, G., "Turbulent Closure and the Modeling of Fire by Using Computational Fluid Dynamics," *Phil. Trans. Roy. Soc. Lond. A* 356, 2835-2854 (1998).	Fire Modeling Turbulence/ Kinetics Soot/Radiation CFD Closure Methods
80148.	Heskestad, G., "Dynamics of the Fire Plume," *Phil. Trans. Roy. Soc. Lond. A* 356, 2815-2833 (1998).	Fire Plumes Turbulent Buoyant Air Entrainment Wind Effects Modeling Capabilities
(80080)	Modeling, H_2/Air/Inert Particles, Size, Gravity Effects	Dust/Flame Interactions
80149.	Vedarajan, T.G., J. Buckmaster and P. Ronney, "Two-Dimensional Failure Waves and Ignition Fronts in Premixed Combustion," *Int. Symp. Combust.* 27, 537-544 (1998).	Edge Flames Premixed Speeds Theory
80150.	Bennett, B.A.V., and M.D. Smooke, "Local Rectangular Refinement with Application to Axisymmetric Laminar Flames," *Combust. Theory Modeling* 2, 221-258 (1998).	Bunsen/ Diffusion Flames Modeling Gridding Method
80151.	Bollig, M., A. Linan, A.L. Sanchez and F.A. Williams, "A Simplified Approach to the Numerical Description of Methane/Air Diffusion Flames," *Int. Symp. Combust.* 27, 595-603 (1998).	Diffusion Flames CH_4/Air Reduced Kinetic Scheme Description
80152.	Mohammed, R.K., M.A. Tanoff, M.D. Smooke, A.M. Schaffer and M.B. Long, "Computational and Experimental Study of a Forced, Time-Varying, Axisymmetric, Laminar Diffusion Flame," *Int. Symp. Combust.* 27, 693-702 (1998).	Diffusion Flame Laminar CH_4/Air Acoustic Forcing SRS,PIV CH* Emission Measurements Modeling

80153. Chen, Y.-c., and J.-Y. Chen, "Fuel-Dilution Effect on Differential Molecular Diffusion in Laminar Hydrogen Diffusion Flames," *Combust. Theory Modeling* 2, 497-514 (1998).

Diffusion Flames
$H_2/N_2/O_2$
Counterflow
Differential
Diffusional Effects

80154. Frouzakis, C.E., J. Lee, A.G. Tomboulides and K. Boulouchos, "Two-Dimensional Direct Numerical Simulation of Opposed-Jet Hydrogen/Air Diffusion Flame," *Int. Symp. Combust.* 27, 571-577 (1998).

Diffusion Flame
Structure
H_2/Air
Opposed Jets

80155. Khokhlov, A.M., E.S. Oran, A.Yu. Chtchelkanova and J.C. Wheeler, "Interaction of a Shock with a Sinusoidally Perturbed Flame," *Combust. Flame* 117, 99-116 (1999).

Flame/Shock
Interactions
C_2H_2/Air
Energy Release
Increase
Modeling

80156. Johnson, R.G., A.C. McIntosh and J. Brindley, "Evolution of a Fast Flame Behind an Induction Zone," *Shock Waves* 6, 225-231 (1996).

Shock Wave
Propagation
Induction Zone
Feedback Model

80157. Daou, J., and A. Linan, "The Role of Unequal Diffusivities in Ignition and Extinction Fronts in Strained Mixing Layers," *Combust. Theory Modeling* 2, 449-477 (1998).

Propagation
Strained
Mixing Layers
Thermo-Diffusive
Model

80158. Daou, J., and A. Linan, "Triple Flames in Mixing Layers with Nonunity Lewis Numbers," *Int. Symp. Combust.* 27, 667-674 (1998).

Triple Flame
Propagation
Nonuniform
Mixtures
Theory

80159. Ern, A., and V. Giovangigli, "Thermal Diffusion Effects in Hydrogen/Air and Methane/Air Flames," *Combust. Theory Modeling* 2, 349-372 (1998).

Propagation
CH_4/Air
H_2/Air
Thermal Diffusion
Effects

80160. Christiansen, E.W., C.J. Sung and C.K. Law, "Pulsating Instability in Near-Limit Propagation of Rich Hydrogen/Air Flames," *Int. Symp. Combust.* 27, 555-562 (1998).

Propagation
Rich H_2/Air
Instabilities
Transport/Kinetics
Simulations

80161. Takahashi, F., W.J. Schmoll and V.R. Katta, "Attachment Mechanisms of Diffusion Flames," *Int. Symp. Combust.* 27, 675-684 (1998).

Diffusion Flame
Burner Attachment
Stabilization
PIV Flowfields
Mechanism

80162.	Blanchard, J.N., Y. Brune and A. Merlen, "Influence of a Counter Rotating Vortex Pair on the Stability of a Jet in a Crossflow: An Experimental Study by Flow Visualizations," *Experiments Fluids* 26, 63-74 (1999).	Stabilization Transverse Jet/ Crossflow Flow Visualization
80163.	Kendrick, D., G. Herding, P. Scouflaire, C. Rolon and S. Candel, "Effect of Recess on Cryogenic Flame Stabilization," *Compt. Rendus Acad. Sci., Paris, Ser. II, b. Mecanique, Physique, Chemie, Astronomie* 326, 111-116 (1998).	Stabilization H_2/Liquid O_2 OH Flame Structure Tomographic Measurements
80164.	Kim, J.S., "On the Onset Condition of Fast-Time Instability in Linan's Premixed Flame Regime," *Combust. Theory Modeling* 2, 273-282 (1998).	Instabilities Premixed Flame Theory Reanalysis
80165.	Sohn, C.H., S.H. Chung and J.S. Kim, "Instability-Induced Extinction of Diffusion Flames Established in the Stagnant Mixing Layer," *Combust. Flame* 117, 404-412 (1999).	Instabilities Diffusion Flame Modeling
80166.	Richards, G.A., and M.C. Janus, "Characterization of Oscillations During Premix Gas Turbine Combustion," Presented Originally as Paper 97-GT-244 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 294-302 (1998).	Oscillations Gas Turbine Premixed Natural Gas/Air Characteristics
(80483)	Dump Combustor, Diode Laser Absorption of H_2O, Temperatures, Adaptive Feedback Method	Combustion Control
80167.	Seume, J.R., N. Vortmeyer, W. Krause, J. Hermann, C.-C. Hantschk, P. Zangl, S. Gleis, D. Vortmeyer and A. Orthmann, "Application of Active Combustion Instability Control to a Heavy Duty Gas Turbine," Presented Originally as Paper 97-AA-119 at the *ASME ASIA '97 Congress and Exhibition*, Held September 1997, *J. Eng. Gas Turb. Power, Trans. ASME* 120, 721-726 (1998).	Instability Control Gas Turbines Active Fuel Flow Feedback Method
80168.	Bui, P.-A., D.G. Vlachos and P.R. Westmoreland, "On the Local Stability of Multiple Solutions and Oscillatory Dynamics of Spatially Distributed Flames," *Combust. Flame* 117, 307-322 (1999).	Oscillatory Combustion Methodology Stability Stationary Solutions H_2/Air
80169.	Brown, T.M., R.W. Pitz and C.J. Sung, "Oscillatory Stretch Effects on the Structure and Extinction of Counterflow Diffusion Flames," *Int. Symp. Combust.* 27, 703-710 (1998).	Extinction Counterflow Diffusion Flames CH_4,N_2/Air Oscillatory Stretch Effects 2-D PLIF,OH

80170. Yoshida, K., and T. Takagi, "Transient Local Extinction and Re-ignition Behavior of Diffusion Flames Affected by Flame Curvature and Preferential Diffusion," *Int. Symp. Combust.* 27, 685-692 (1998).

Extinction
Re-ignition
H_2,N_2/Air
Counterflow
Diffusion Flames
Impinging Microjet
2-D Temperature
Mapping

80171. Lee, S.D., D.H. Chung and S.H. Chung, "Local Equilibrium Temperature as a Measure of Stretch and Preferential Diffusion Effects in Counterflow H_2/Air Premixed Flames," *Int. Symp. Combust.* 27, 579-585 (1998).

Extinction
Premixed
H_2/Air
Stretch
Diffusional Effects
Local Equilibrium
T Concept

80172. Wierzba, I., and B.B. Ale, "Effects of Temperature and Time of Exposure on the Flammability Limits of Hydrogen/Air Mixtures," *Int. J. Hydrogen Energy* 23, 1197-1202 (1998).

Flammability
Limits
H_2/Air
≤350 °C

80173. Shebeko, Yu.N., A.Ya. Korolchenko, E.D. Zamishevski, A.V. Trunev, V.Yu. Navzenya and A.A. Zaitzev, "An Experimental Investigation of Blow-Out Limits for Hydrogen/Diluent Diffusion Flames," *Combust. Flame* 117, 438-440 (1999).

Blow-off Limits
H_2/N_2(H_2O)
Diffusion Flames
Measurements

12. TURBULENCE

(See Section 14 for Flowfield and Visualization)

80174. Hwang, R.R., and S.-Y. Jaw, "Second-Order Closure Turbulence Models: Their Achievements and Limitations," *Proc. Natl. Sci. Council, Taiwan, A. Phys. Sci. Eng.* 22, 703-722 (1998).

Turbulence
Second Order
Closure Models
Differences

80175. Cook, A.W., and W.K. Bushe, "A Subgrid-Scale Model for the Scalar Dissipation Rate in Nonpremixed Combustion," *Phys. Fluids* 11, 746-748 (1999).

Turbulent
Combustion
Scalar
Dissipation Rate
Model

80176. Zimont, V., W. Polifke, M. Bettelini and W. Weisenstein, "An Efficient Computational Model for Premixed Turbulent Combustion at High Reynolds Numbers Based on a Turbulent Flame Speed Closure," Presented Originally as Paper 97-GT-395 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 526-532 (1998).

Turbulent
Premixed
Combustion
High Reynolds
Number
Model

80177.	Hoffmann, S., B. Lenze and H. Eickhoff, "Results of Experiments and Models for Predicting Stability Limits of Turbulent Swirling Flames," Presented Originally as Paper 97-GT-396 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 311-316 (1998).	Turbulent Swirling Flames Lean Stability Limits Predictive Model
80178.	Koutmos, P., "Simulations of Turbulent Methane Jet Diffusion Flames with Local Extinction Effects," *Fluid Dyn. Res.* 24, 103-119 (1999).	Turbulent Jet Flames Large Eddy Simulation Model CH_4/Air
(80148)	Turbulent, Air Entrainment, Wind Effects, Modeling Capabilities	Buoyant Fire Plumes
(80147)	Fire Modeling, Kinetics, Soot/Radiation, CFD, Closure Methods	Turbulence Effects
(80083)	Hollow Cone Spray/Heated Air Stream, Vaporization, PDA, Modeling	Turbulent Flows
80179.	Kagan, L., G. Sivashinsky and G. Makhviladze, "On Flame Extinction by a Spatially Periodic Shear Flow," *Combust. Theory Modeling* 2, 399-404 (1998).	Turbulence Shear Flow Extinction Model
80180.	Helenbrook, B.T., and C.K. Law, "The Role of Landau-Darrieus Instability in Large Scale Flows," *Combust. Flame* 117, 155-169 (1999).	Turbulent Propagation Instability Mechanism
80181.	Bohn, D., G. Deutsch and U. Kruger, "Numerical Prediction of the Dynamic Behavior of Turbulent Diffusion Flames," Presented Originally as Paper 96-GT-133 at the *41st International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Birmingham UK, June 1996, *J. Eng. Gas Turbines, Trans. ASME* 120, 713-720 (1998).	Turbulent Diffusion Flames Oscillation Instabilities Predictive Model
80182.	Boineau, P., and Y. Gervais, "Turbulent Flame Acoustic Power Spectrum Determination," *Compt. Rendus Acad. Sci., Paris, Ser. II, b. Mecanique, Physique, Chemie, Astronomie* 326, 747-754 (1998).	Turbulent Combustion Noise Spectrum Model
80183.	Truffaut, J.-M., G. Searby and L. Boyer, "Sound Emission by Non-Isomolar Combustion at Low Mach Numbers," *Combust. Theory Modeling* 2, 423-428 (1998).	Turbulent Acoustic Emission Molar Expansion Role
80184.	Alshaalan, T.M., and C.J. Rutland, "Turbulence, Scalar Transport, and Reaction Rates in Flame/Wall Interaction," *Int. Symp. Combust.* 27, 793-799 (1998).	Turbulent Flame Near Wall Interactions Flowfield Modifications Modeling

80185. Mazumder, S., and M.F. Modest, "A Probability Density Function Approach to Modeling Turbulence-Radiation Interactions in Nonluminous Flames," *Int. J. Heat Mass Transfer* 42, 971-991 (1999).

Turbulence/ Radiation Interactions
CH_4/Air
Diffusion Flame
Model

80186. Khokhlov, A.M., E.S. Oran and G.O. Thomas, "Numerical Simulation of Deflagration-to-Detonation Transition: The Role of Shock-Flame Interactions in Turbulent Flames," *Combust. Flame* 117, 323-339 (1999).

Turbulent Flame/Shock Interactions
C_2H_2/Air
Deflagration/ Detonation
Modeling

80187. Ju, Y., A. Shimano and O. Inoue, "Vorticity Generation and Flame Distortion Induced by Shock Flame Interaction," *Int. Symp. Combust.* 27, 735-741 (1998).

Vorticity Generation
H_2/Air Flame
Shock Propagation
Flame Distortion
Modeling

80188. Kalinnikov, V.T., and A.F. Gutsol, "Insulation of a Gaseous Flame in a Reciprocal Vortex," *Dokl. Phys.* 43, 302-305 (1998).

Reciprical Vortex
Stabilized Flame
Enhanced Thermal Efficiencies
Reduced NO_x

80189. Louch, D.S., and K.N.C. Bray, "Vorticity and Scalar Transport in Premixed Turbulent Combustion," *Int. Symp. Combust.* 27, 801-810 (1998).

Flame/Vortex Interactions
Turbulent Structures
Modeling

80190. Patnaik, G., and K. Kailasanath, "A Computational Study of Local Quenching in Flame/Vortex Interactions with Radiative Losses," *Int. Symp. Combust.* 27, 711-717 (1998).

Flame/Vortex Interactions
Lean CH_4/Air
Local Quenching
Radiative Loss
Modeling

80191. Katta, V.R., C.D. Carter, G.J. Fiechtner, W.M. Roquemore, J.R. Gord and J.C. Rolon, "Interaction of a Vortex with a Flat Flame Formed Between Opposing Jets of Hydrogen and Air," *Int. Symp. Combust.* 27, 587-594 (1998).

Flame/Vortex Interactions
Quenching Patterns
H_2,N_2/Air
OH,LIF

80192. Thevenin, D., P.H. Renard, J.C. Rolon and S. Candel, "Extinction Processes During a Nonpremixed Flame/Vortex Interaction," *Int. Symp. Combust.* 27, 719-726 (1998).

Flame/Vortex Interactions
H_2/Air
Extinction
Mixing,Strain Roles

80193. Renard, P.-H., J.C. Rolon, D. Thevenin and S. Candel, "Investigations of Heat Release, Extinction, and Time Evolution of the Flame Surface, for a Nonpremixed Flame Interacting with a Vortex," *Combust. Flame* 117, 189-205 (1999).

Flame/Vortex Interactions
H_2/Air
OH,PLIF
Extinctions

80194. Saxena, V., and S.B. Pope, "PDF Simulations of Turbulent Combustion Incorporating Detailed Chemistry," *Combust. Flame* 117, 340-350 (1999).

Turbulent Combustion
Detailed Kinetics
PDF Calculations
Method

80195. Mallampalli, H.P., T.H. Fletcher and J.Y. Chen, "Evaluation of CH_4/NO_x Reduced Mechanisms Used for Modeling Lean Premixed Turbulent Combustion of Natural Gas," *J. Eng. Gas Turb. Power, Trans. ASME* 120, 703-712 (1998).

Turbulent Combustion
CH_4/Air
Kinetic Modeling
Reduced Schemes
Gas Turbines
NO_x Predictions

80196. Barlow, R.S., N.S.A. Smith, J.-Y. Chen and R.W. Bilger, "Nitric Oxide Formation in Dilute Hydrogen Jet Flames: Isolation of the Effects of Radiation and Turbulence-Chemistry Submodels," *Combust. Flame* 117, 4-31 (1999).

Turbulent
H_2/O_2/He
Kinetic/ Radiative Submodels
NO Formation

80197. Chen, Y.-C., and M.S. Mansour, "Investigation of Flame Broadening in Turbulent Premixed Flames in the Thin-Reaction Zones Regime," *Int. Symp. Combust.* 27, 811-818 (1998).

Turbulent
3-D Flame Structure
2-D 2-Plane Rayleigh
Temperatures
Preheat Zone Thickness

80198. Mansour, M.S., N. Peters and Y.-C. Chen, "Investigation of Scalar Mixing in the Thin Reaction Zones Regime Using a Simultaneous CH LIF/Rayleigh Laser Technique," *Int. Symp. Combust.* 27, 767-773 (1998).

Turbulent
CH_4/Air
Highly Stretched
2-D Rayleigh/ LIF,CH
Temperature Measurements

80199.	Soika, A., F. Dinkelacker and A. Leipertz, "Measurement of the Resolved Flame Structure of Turbulent Premixed Flames with Constant Reynolds Number and Varied Stoichiometry," *Int. Symp. Combust.* 27, 785-792 (1998).	Turbulent CH_4/Air Planar Rayleigh 3-D Temperature Gradients Measurements
80200.	Gagnepain, L., C. Chauveau and I. Gokalp, "A Comparison between Dynamic and Scalar Timescales in Lean Premixed Turbulent Flames," *Int. Symp. Combust.* 27, 775-787 (1998).	Turbulent Lean CH_4/Air LDV Mie,Rayleigh Timescale Measurements
80201.	Frank, J.H., and R.S. Barlow, "Simultaneous Rayleigh, Raman, and LIF Measurements in Turbulent Premixed Methane/Air Flames," *Int. Symp. Combust.* 27, 759-766 (1998).	Turbulent CH_4/Air Rayleigh,Raman T,Major Species LIF,CO,NO,OH Measurements
80202.	Dinkelacker, F., A. Soika, D. Most, D. Hofmann, A. Leipertz, W. Polifke and K. Dobbeling, "Structure of Locally Quenched Highly Turbulent Lean Premixed Flames," *Int. Symp. Combust.* 27, 857-865 (1998).	Turbulent CH_4/Air Swirl Stabilized 2-D T,OH,LIF Flame Structure Quenching
80203.	Chen, J.H., and H.G. Im, "Correlation of Flame Speed with Stretch in Turbulent Premixed Methane/Air Flames," *Int. Symp. Combust.* 27, 819-826 (1998).	Turbulent CH_4/Air Flame Speed/ Stretch Correlation Modeling
(80514)	Turbulent Flamelet Surfaces, Monitoring Method	Laser Tomography
80204.	Sinibaldi, J.O., C.J. Mueller and J.F. Driscoll, "Local Flame Propagation Speeds Along Wrinkled, Unsteady, Stretched Premixed Flames," *Int. Symp. Combust.* 27, 827-832 (1998).	Turbulent Wrinkled Flames Displacement Speed Parameter PIV,Shadowgraph
80205.	Peters, N., P. Terhoeven, J.H. Chen and T. Echekki, "Statistics of Flame Displacement Speeds from Computations of 2-D Unsteady Methane/Air Flames," *Int. Symp. Combust.* 27, 833-839 (1998).	Turbulent CH_4/Air Displacement Speed Contributing Mechanisms

80206. Renou, B., A. Boukhalfa, D. Puechberty and M. Trinite, "Effects of Stretch on the Local Structure of Freely Propagating Premixed Low Turbulent Flames with Various Lewis Numbers," *Int. Symp. Combust.* 27, 841-847 (1998).

Turbulent
CH_4,C_3H_8,H_2/Air
PIV/
Laser Tomography
Displacement
Speeds
Strain Rates

80207. Bradley, D., P.H. Gaskell and X.J. Gu, "The Modeling of Aerodynamic Strain Rate and Flame Curvature Effects in Premixed Turbulent Combustion," *Int. Symp. Combust.* 27, 849-856 (1998).

Turbulent
Burning Velocities
C_3H_8/Air
Strain,Curvature
Modeling

80208. Kalt, P.A.M., J.H. Frank and R.W. Bilger, "Laser Imaging of Conditional Velocities in Premixed Propane/Air Flames by Simultaneous OH PLIF and PIV," *Int. Symp. Combust.* 27, 751-758 (1998).

Turbulent
Velocities
C_3H_8/Air
PIV,PLIF OH
Measurements

13. DETONATIONS/EXPLOSIONS

80209. Shouman, A.R., and S.A. El-Sayed, "Accounting for Reactant Consumption in the Thermal Explosion Problem. IV. Numerical Solution of the Arrhenius Problem," *Combust. Flame* 117, 422-428 (1999).

Thermal Explosions
Arrhenius
Kinetics
Numerical Solver
Modeling

80210. Short, M., and A.K. Kapilo, "Blow-up in Semilinear Parabolic Equations with Weak Diffusion," *Combust. Theory Modeling* 2, 283-291 (1998).

Thermal Runaway
Blow-up Kinetics
Mathematical
Modeling

80211. Berkenbosch, A.C., E.F. Kaasschieter and R. Klein, "Detonation Capturing for Stiff Combustion Chemistry," *Combust. Theory Modeling* 2, 313-348 (1998).

Detonation Wave
Stiff Integration
Method

80212. Williams, D.N., L. Bauwens and E.S. Oran, "A Numerical Study of the Mechanisms of Self-reignition in Low Overdrive Detonations," *Shock Waves* 6, 93-110 (1996).

Detonations
Instabilities
Re-ignition
Theory

80213. Brailovsky, I., and G.I. Sivashinsky, "Momentum Loss as a Mechanism for Deflagration-to-Detonation Transition," *Combust. Theory Modeling* 2, 429-447 (1998).

Deflagration/
Detonation
Transitions
Propagation
Porous Medium

80214.	Alekseev, V.I., S.B. Dorofeev and V.P. Sidorov, "Direct Initiation of Detonations in Unconfined Gasoline Sprays," *Shock Waves* 6, 67-71 (1996).	Detonations Gasoline Spray Unconfined Clouds Initiation Energies
(80091)	Fuel Spray, Propagation, Numerical Modeling	Detonation Waves
80215.	Presles, H.N., D. Desbordes, M. Guirard and C. Guerraud, "Gaseous Nitromethane and Nitromethane/Oxygen Mixtures: A New Detonation Structure," *Shock Waves* 6, 111-114 (1996).	Detonations CH_3NO_2 CH_3NO_2/O_2 Cellular Structures
80216.	Legendre, J.-F., M. Giraud and P. Bauer, "Detonation Properties of Dense Methane/Oxygen/Diluent Gaseous Mixtures: Application to Ram Accelerators," *Shock Waves* 8, 267-273 (1998).	Detonations $CH_4/O_2/CO_2, N_2, He$ Limits,Velocities Pressures Measurements
80217.	Sochet, I., M. Aminallah and J. Brossard, "Detonability of Fuel/Oxygen and Fuel/Air Mixtures," *Shock Waves* 7, 163-174 (1997).	Detonations $CH_4, C_2H_2/O_2$, Air C_3H_8/O_2, Air Critical Energies
80218.	Takita, K., and T. Niioka, "On Detonation Behavior of Mixed Fuels," *Shock Waves* 6, 61-66 (1996).	Detonations $CH_4, C_3H_8/H_2$ CH_4/C_4H_{10} Mixed Fuels Velocities Induction Times
(80186)	Modeling, Turbulent C_2H_2/Air/Shock Interactions	Deflagration/ Detonations
80219.	Bolk, J.W., and K.R. Westerterp, "Influence of Hydrodynamics on the Upper Explosion Limit of Ethene/Air/Nitrogen Mixtures," *AIChE J.* 45, 124-144 (1999).	C_2H_4/Air/N_2 Upper Explosion Limits Gas Flow Effects
80220.	Fehlings, M., D. Konig and H. Vogel, "Explosion Limits of Propene/Oxygen/Alkane Mixtures and their Reactivity with Bi/Mo Mixed Oxide Systems," *Chem. Technik* 50, 241-245 (1998).	$C_3H_6/O_2/M$ Explosion Limits $M = CH_4, C_3H_8, N_2$ Measurements
80221.	Dorofeev, S.B., V.P. Sidorov, M.S. Kuznetsov, A.E. Dvoinishnikov, V.I. Alekseev and A.A. Efimenko, "Air Blast and Heat Radiation from Fuel-Rich Mixture Detonations," *Shock Waves* 6, 21-28 (1996).	Detonations C_3H_8/Air Fireballs Air Blast Scaling Parameters

80222. Dorofeev, S.B., A.V. Bezmelnitsin, V.P. Sidorov, J.G. Yankin and I.D. Matsukov, "Turbulent Jet Initiation of Detonation in Hydrogen/Air Mixtures," *Shock Waves* 6, 73-78 (1996).

Detonations
H_2/Air
Turbulent Jet
Hot Gas
Initiation

80223. Leblanc, J.E., M.H. Lefebvre and T. Fujiwara, "Detailed Flowfields of a Ram Accelerator Device in H_2/O_2 Full Chemistry," *Shock Waves* 6, 85-92 (1996).

Detonations
Hypersonic Flows
Ram Accelerator
H_2/O_2
Modeling

14. FLOW PHENOMENA/VELOCITIES/DIFFUSION

(See also Section 5 for Spray Flowfields and Velocities and Section 12 for Turbulent Flowfields)

80224. Birouk, M., and A.K. Gupta, "Swirl Distribution Effects on the Structure of Lean Premixed Flames using PLIF Diagnostics," *J. Heat Transfer, Trans ASME* 120, 541 (1998).

Flow Visualization
CH_4/Air
Swirl Effects
PLIF,OH
Images

(80162) Stabilization, Transverse Jet/Crossflow

Flow Visualization

80225. Wendt, M.N., and R.J. Stalker, "Transverse and Parallel Injection of Hydrogen with Supersonic Combustion in a Shock Tunnel," *Shock Waves* 6, 53-59 (1996).

Supersonic Flow
H_2 Injection
Transverse/
Parallel Flow
Effects

(80223) Ram Accelerator Flowfields, Detonations, H_2/O_2 Modeling

Hypersonic Flows

80226. Luff, J.D., T. Drouillard, A.M. Rompage, M.A. Linne and J.R. Hertzberg, "Experimental Uncertainties Associated with Particle Image Velocimetry Based Vorticity Algorithms," *Experiments Fluids* 26, 36-54 (1999).

PIV
Vorticity
Algorithm
Uncertainties

(80161) Burner Attachment Stabilization, Diffusion Flame, Mechanism

PIV Flowfields

80227. Vihinen, I., J.R. Gord, J.M. Donbar, R.D. Hancock, W.M. Roquemore, G.J. Fiechtner, C.D. Carter, K.D. Grinstead Jr, V.R. Katta and J.C. Rolon, "Flame-Vortex Interactions in a Counterflow Burner," *J. Heat Transfer, Trans ASME* 120, 540 (1998).

Flow Visualization
Flame/Vortex
Interactions
Counterflow Burner
PLIF,OH
Images

80228. Renard, P.-H., J.C. Rolon, D. Thevenin and S. Candel, "Wrinkling, Pocket Formation and Double Premixed Flame Interaction Processes," *Int. Symp. Combust.* 27, 659-666 (1998).

Counterflow
Double
Premixed Flame
Vortex Ring
Interactions
C_3H_8/Air
Structure

80229. Huang, R.F., and S.M. Wang, "Characteristic Flow Modes of Wake-Stabilized Jet Flames in a Transverse Air Stream," *Combust. Flame* 117, 59-77 (1999).

Flowfields
Jet Flames
Transverse Air
LDV

80230. Watson, K.A., K.M. Lyons, J.M. Donbar and C.D. Carter, "Scalar and Velocity Field Measurements in a Lifted CH_4/Air Diffusion Flame," *Combust. Flame* 117, 257-271 (1999).

Flowfield
Leading Edge
Lifted Jet
Diffusion Flame
CH_4/Air
PIV
PLIF/CH,OH

80231. Shu, Z., B.J. Krass, C.W. Choi, S.K. Aggarwal, V.R. Katta and I.K. Puri, "An Experimental and Numerical Investigation of the Structure of Steady Two-Dimensional Partially Premixed Methane/Air Flames," *Int. Symp. Combust.* 27, 625-632 (1998).

Partially Premixed
CH_4/Air
3-Slot Burner
Mixing Structure
PIV Velocities

80232. Ma, L.-Z., and J. Chomiak, "Asymptotic Flame Shapes and Speeds of Hydrodynamically Unstable Laminar Flames," *Int. Symp. Combust.* 27, 545-553 (1998).

Flame Speeds
Shapes
Laminar Flows
Baroclinic
Instabilities
Theory

(80159) CH_4, H_2/Air Propagation

Thermal Diffusion
Effects

80233. Ishizuka, S., T. Hamasaki, K. Koumura and R. Hasegawa, "Measurements of Flame Speeds in Combustible Vortex Rings: Validity of the Back-Pressure Drive Flame Propagation Mechanism," *Int. Symp. Combust.* 27, 727-734 (1998).

Flame Speeds
Vortex Axis
CH_4/Air
Propagation
Mechanism
Validation

80234. Leylegian, J.C., C.K. Law and H. Wang, "Laminar Flame Speeds and Oxidation Kinetics of Tetrachloromethane," *Int. Symp. Combust.* 27, 529-536 (1998).

Laminar
Flame Speeds
CH_4/CCl_4/Air
Measurements
Modeling

80235.	Vagelopoulos, C.M., and F.N. Egolfopoulos, "Direct Experimental Determination of Laminar Flame Speeds," *Int. Symp. Combust.* 27, 513-519 (1998).	Laminar Flame Speeds New Methodology LDV CH_4,C_2H_6,C_3H_8/Air
(80216)	$CH_4/O_2/CO_2$, N_2, He, Limits, Pressures, Measurements	Detonation Velocities
(80218)	CH_4, C_3H_8/H_2; CH_4/C_4H_{10} Mixed Fuels, Induction Times	Detonation Velocities
80236.	Davis, S.G., and C.K. Law, "Laminar Flame Speeds and Oxidation Kinetics of *iso*-Octane/Air and *n*-Heptane/Air Flames," *Int. Symp. Combust.* 27, 521-527 (1998).	Laminar Flame Speeds C_3H_6,*i*-C_4H_8/Air *n*-C_7H_{16},*i*-C_8H_{18}/Air Measurements Model
(80081)	Dust Flames, Propagation, Heat Transfer Models	Burning Velocities
(80269)	Diffusion Coefficients, Heterogeneous Uptake Coefficient Measurements	$ClNO_2$/He,N_2

15. IONIZATION

(See also Section 40 for Dynamics of Ion-Molecule Reactions, Section 43 for Ion P.E. Curves and Surfaces, Section 44 for Ionic Structures and Section 46 for Thermochemical Values)

80237.	Taylor, W.S., E.M. Spicer and D.F. Barnas, "Metastable Metal Ion Production in Sputtering dc Glow Discharge Plasmas: Characterization by Electronic State Chromatography," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 643-650 (1999).	Metal Ions Metastable Excited States Discharge Sputtering Characterization
80238.	Ulybyshev, K.E., "Electronic Structure of the Combustion Front in a Homogeneous Methane/Air Mixture," *Fluid Dyn., Russia* 33, 1-4 (1998).	Flame Ions Combustion Front Propagation Role Modeling
(80468)	Microliter Sample Monitoring Method	Microwave Plasma Mass Analysis
(80470)	Laser Ablation Calibration Method	ICP/MS
(80127)	Laser Enhanced Ionization, C_2H_2/Air Flame Temperatures, 2-Step Pumping	Al,Ga

80239. Scott, G.B.I., D.A. Fairley, C.G. Freeman, M.J. McEwan and V.G. Anicich, "$C_mH_n^+$ Reactions with Atomic and Molecular Nitrogen: An Experimental Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1073-1077 (1999).

$C_mH_n^+ + N,N_2$
m=1-6,n=0-6
Rate Constants
Ion Products

80240. Le Padellec, A., J.B.A. Mitchell, A. Al-Khalili, H. Danared, A. Kallberg, A. Larson, S. Rosen, M. af Ugglas, L. Vikor and M. Larsson, "Storage Ring Measurements of the Dissociative Recombination and Excitation of the Cyanogen Ion $CN^+(X^1\Sigma^+$ and $a^3\Pi,v=0)$," *J. Chem. Phys.* 110, 890-901 (1999).

$CN^+(a,X) + e^-$
Dissociative Recombination
Rate Constants
Branching Ratios
P.E. Curves

80241. Tsuji, M., E. Oda, M. Nakamura and Y. Nishimura, "Formation of $CO(d^3\Delta_i$, $a'^3\Sigma^+)$ by Dissociative Ion-Ion Neutralization Reaction of CO_2^+ with $C_6F_6^-$ in the Helium Flowing Afterglow," *Chem. Lett. Jpn.* 413-414 (1998).

$CO_2^+ + C_6F_6^-$
Neutralization
CO(d,a′-a)
Spectral Emission
Product Vibrational Distributions

(80386) FTIR Spectra, Frequencies, Matrix Study

$CO_2^-,(CO_2)_2^-$

(80487) Cavity Ringdown Absorption, Pulse Slit Nozzle Discharge, Sensitivities

$C_2^-(B\text{-}X)$
$C_6H_2^+(^2\Pi\text{-}X)$

80242. Hayakawa, S., M. Takahashi, K. Arakawa and N. Morishita, "Definitive Evidence for the Existence of a Long-Lived Vinylidene Radical Cation, $H_2C=C^+$," *J. Chem. Phys.* 110, 2745-2748 (1999).

$CH_2C^+(X^2B_1)$
Formation
Lifetime
Measurement

(80776) Chemiionization Energetics, Structural Calculations

$CH_3C + O$

(80584) fs MPD/MPI, Product Ions, Fragmentations, Measurements

c-C_3H_6,C_6H_6
c-C_6H_{12}

(80629) Unimolecular Dissociation, Rate Constants, Channels, Calculations

$C_3H_8^+$

80243. Hirose, Y., I. Ishikawa, S. Sasaki, K. Nagaseki, Y. Saito and S. Suganomata, "Positive Ions in Radiofrequency Discharge Plasmas of C_4F_8/Ar and C_4F_8/O_2 Mixtures," *Jpn. J. Appl. Phys.* 37, 5730-5734 (1998).

$C_nF_m^+$,COF_n^+
Ions
C_4F_8/O_2(Ar)
Discharges

(80633) Unimolecular Isomerization, IP($C_2H_5COOCH_3$), $\Delta H_f(C_2H_5CO^+)$, Channels, Measurements

$C_2H_5COOCH_3^+$

80244. Knighton, W.B., T.M. Miller, A.A. Viggiano, R.A. Morris and J.M. Van Doren, "Gas Phase Reactions of Oxide and Superoxide Radical Anions with C_6F_6," *J. Chem. Phys.* 109, 9632-9633 (1998).

$C_6F_6 + O_2^-,O^-$
$C_6F_6^- + O_2$
Rate Constants
Branching Ratios

(80469) Automobile Exhaust Monitor

Aromatics
Photoionization/
Mass Analysis

(80395)	Absorption Spectrum, D-Isotopes, Constants, Geometry	$C_6H_2^+$(A-X)
(80635)	Unimolecular Dissociation, X=Cl, Br, I, Product X Atom Kinetic Energies, Measurements	$C_6H_5X^+$
(80396)	Isomers, Infrared/Photoinduced Rydberg Ionization Spectrum, ν_{OH} Frequencies, Ground/Low-lying States	1,3-$C_6H_4(OH)_2^+$
(80370)	Spectroscopy, Structure, Energies, Review	C_n^+,C_n^-,C_n
80245.	Foltin, V., M. Foltin, S. Matt, P. Scheier, K. Becker, H. Deutsch and T.D. Mark, "Electron Impact Ionization of C_{60} Revisited: Corrected Absolute Cross Section Functions," *Chem. Phys. Lett.* 289, 181-188 (1998).	$C_{60}+e^-$ Ionization Cross Sections Product Ions
80246.	Mazurek, U., D. Schroder and H. Schwarz, "Generation and Reactivity of Chromium Fluoride Cations (CrF_n^+, n=0-4) in the Gas Phase," *Collect. Czech. Chem. Commun.* 63, 1498-1512 (1998).	$CrF_n^+ + RH$ Reactivities n=1-4 C_1-C_4 Alkanes Product Ions
(80459)	Transition Probabilities, Calculations	Cu^+
(80408)	FTIR Spectra, Frequencies, Laser Ablated Fe/CO Matrix Study	$Fe(CO)_n^-$,n=1-3
80247.	Hassouni, K., A. Gicquel and M. Capitelli, "The Role of Dissociative Attachment from Rydberg States in Enhancing H^- Concentration in Moderate an Low Pressure H_2 Plasma Sources," *Chem. Phys. Lett.* 290, 502-508 (1998).	$H_2^* + e^-$ Rydberg State Attachment H^- Formation
(80413)	Assignments, H_2 PFI/PES Spectrum, Rotational Constants	H_2^+(v=0,2,9,11)
80248.	Marziano, N.C., A. Tomasin, C. Tortato and P. Isandelli, "The Problem of Acidity in Concentrated Aqueous Solutions of Sulfuric Acid," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 2535-2540 (1998).	$H_2SO_4/H^+ + HSO_4^-$ $HSO_4^-/H^+ + SO_4^{2-}$ Solution Equilibria
80249.	Ishida, T., and H. Katagiri, "Corrigendum to Spin-Orbit Effects on Penning Ionization: $Ar + He(2^3S) \rightarrow Ar^+(^2P_{3/2},^2P_{1/2}) + He + e^-$: An ab Initio and Trajectory Study [*Chem. Phys. Lett.* 274, 293-298 (1997)]," *ibid.* 290, 296 (1998).	$He(2^3S) + Ar$ Penning Ionization Calculations Erratum
80250.	Mastwijk, H.C., M. van Rijnbach, J.W. Thomsen, P. van der Straten and A. Niehaus, "Photo Induced Collisions with Laser Cooled He* Atoms," *Eur. Phys. J. D* 4, 131-137 (1998).	He* + He* Penning/ Associative Ionizations Optical Trap Low Temperature
(80443)	Penning Ionization Cross Sections, Energy Dependences, Calculations	$He(2^3S) + N_2$
(80611)	Neutralizations, X=F, Cl, Br, CF_3 Product He* Rydberg State Distributions, Measurements, Modeling	$He^+ + C_6F_5X^-$

(80414)	Rotational Spectrum, Constants, v=0,1	HeD^+
80251.	Brussaard, G.J.H., E. Aldea, M.C.M. van de Sanden, G. Dinescu and D.C. Schram, "Evidence for Charge Exchange Between N^+ and $N_2(A^3\Sigma_u^+)$ in a Low Temperature Nitrogen Plasma," *Chem. Phys. Lett.* 290, 379-384 (1998).	$N^+ + N_2(A)$ Charge Transfer $N_2^+(B)$ Product (B-X) Emission
80252.	Tsuji, M., H. Ishimi, H. Oota, M. Hisano and Y. Nishimura, "The Influence of Vibrational Excitation of $NO^+(X^1\Sigma^+,v)$ on the Formation of NO* by the $NO^+ + C_6F_6^-$ Neutralization Reaction at Thermal Energy," *Bull. Chem. Soc. Jpn .* 72, 227-233 (1999).	$NO^+(v) + C_6F_6^-$ Neutralization NO(D,C,A-X) Product Emission Reactant Vibrational Effects
(80614)	$N_2(v=0,J=40\text{-}90)$, $N_2(v=1)$ Photofragment Anisotropies, $N_2O+h\nu$, Measurements	N_2, REMPI
(80643)	Isomerizations, Catalyzed by Various Neutral Molecules (Ar, HF, CO,N_2, H_2O, H_2, HCl), Energy Barrier Lowering Mechanism	NNH^+,$NNCH_3^+$
80253.	Tsao, C.-C., Y. Wang, R. Napolitano and J. Weiner, "Anisotropy of Optical Suppression in Photoassociative Ionization Collisions within a Slow, Collimated Sodium Atom Beam," *Eur. Phys. J. D* 4, 139-144 (1998).	Na* + Na* Associative Ionization Polarization Anisotropy Effects
(80594)	fs Pump/Probe, NaK^+, Na^+ Channels, P.E. Curves, Pathway Control	NaK,MPI
80254.	Lescop, B., M. Ben Arfa, M. Cherid, G. Fanjoux and E. Kassab, "Penning Ionization Electron Spectroscopy of N_2 with $Ne(^3P_{0,2})$," *J. de Chim. Phys.* 95, 2113-2128 (1998).	$Ne(^3P_{0,2}) + N_2$ Penning Ionization Well Depth $N_2^+(v)$ Product Distribution $N_2^+(A)$ Intermediate
(80465)	Line Strengths, Experiment/Theory Comparisons	$Ne^+(3p\text{-}3d)$
(80615)	$O_3+h\nu$ (276 nm), (3+1), (2+1) Ion Imaging, Product Distributions, Alignments	$O(^1D)$,REMPI
(80428)	PFI-PES Spectra, v′ =0-7, Ion Constants, Predissociation Lifetimes, IP	$O_2^+(B)$-$O_2(X)$ $O_2^+(^2\Sigma_u^-)$-$O_2(X)$
80255.	Antoniotti, P., L. Operti, R. Rabezzana, G. Tonachini and G.A. Vaglio, "Gas Phase Ion Chemistry and ab Initio Theoretical Study of Phosphine. II. Reactions of PH^+ with PH_3," *J. Chem. Phys.* 109, 10853-10863 (1998).	$PH^+ + PH_3$ Rate Constants Product Ions Measurements $\Delta H_f(P_2H_n^+)$,n=0-4 Calculations

80256. Kraemer, W.P., M. Jurek and V. Spirko, "Quantum-Mechanical Studies of Radiative Association Reactions: Formation of HeH^+, NeH^+ and ArH^+," in *Vibration-Rotational Spectroscopy and Molecular Dynamics: Advances in Quantum Chemical and Spectroscopical Studies of Molecular Structures and Dynamics*, D. Papousek, ed., 9 Contributions, 562 pp., *Advanced Ser. Phys. Chem.* 9, 516-553 (1997).

$Rg^+ + H$
Radiative Recombination
Rg = He,Ne,Ar
RgH^+(A-X)
Calculations

80257. Goodings, J.M., and Q.F. Chen, "Chemical Kinetics and Thermodynamics of Tin Ionization in $H_2/O_2/N_2$ Flames and the Proton Affinity of SnO," *Can. J. Chem.* 76, 1437-1446 (1998).

Sn
Flame Chemistry
Sn,SnO,Sn^+
$SnOH^+$ Profiles
PA(SnO)
ΔH_f ,$D_0(SnOH^+)$
$SnOH^+ + e^-$
Rate Constant

(80458) Quenching Rate, Ion Trap

$Sr^+(4^2D_{3/2}) + He$

(80434) ZEKE, PES Spectra, Low-lying States, Constants, Measurements

XeI,XeI^-

16. INHIBITION/ADDITIVES

(80080) H_2/Air/Dust Interactions, Modeling, Size, Gravity Effects

Inert Particles

(80324) Additives, Alkali Emissions Control, Absorption

Alumino-Silicate Clays

(80234) Laminar Flame Speeds, CH_4/CCl_4/Air, Measurements, Modeling

CCl_4 Effects

(80499) CH_4/Air Flames, CCl, CH, NO Species Profiles, LIF Monitoring

CH_3Cl,CH_2Cl_2 Effects

(80344) Reburn Method, NO_x Control, Full/Reduced Kinetic Models

CH_4/NH_3

(80506) CH_4/O_2 Flames, Species Profiles, Sampling, VUV Mass Analyzer, Products, Kinetics

C_2HCl_3 Effects

(80131) CH_4/O_2 Auto-ignition, Kinetic Modeling

$(CH_3)_2O$,C_2H_6
NO_x Effects

(80512) Phosphorus Flame Chemistry, Species Profiles, Kinetic Modeling

$(CH_3)_3PO_3$

(80287) I.C. Engine, Gasoline Additives, Ignition Effects, Hydrocarbon, CO, NO_x Emissions

Furan,p-Cresol

(80295) Soot Control Effects, Diesel Engine

Oxygenated Fuel Additives

(80368) Incinerator Fly Ash, Sample Analysis, 32 Trace Elements, Cl Speciation Effects

Cl Volatilization Efficiencies

(80117)	CuO/TiO_2 Catalytic Oxidation of Soot	Cl^- Effects
(80099)	Boron Particle Combustion, Multiphase Model, Species Profiles, Kinetic Model	F Effects
(80140)	CH_4/C_2H_4 Blend, Ignition, High Strain Rates, Transport/Kinetic Modeling	F_2, H_2 Effects
(80863)	Super-efficient Flame Suppressant Reaction Energetics, ΔH_f(FeH, FeO, FeOH, FeO_2, FeO(OH), $Fe(OH)_2$), Calculations	Fe
(80371)	C_2H_2/Ar Pyrolysis, C_n Nanotube Formation	$Fe(CO)_5$ Effects
(80347)	NO_x, SO_2 Control, Corona Discharge Method, Efficiencies	NH_3 Additive
(80108)	Initiation, Smoldering Combustion, Cellulosic Fabrics	Na,K Effects

17. CORROSION/EROSION/DEPOSITION

(See also Section 22 for Diamond Formation Deposition)

80258. Frenklach, M., "Simulation of Surface Reactions," *Pure Appl. Chem.* 70, 477-484 (1998).

CVD
Surface Chemistry
Theoretical
Descriptive
Approaches

18. GAS/SURFACE INTERACTIONS/BOUNDARY LAYER COMBUSTION

(See also Section 7 for Catalytic Combustion, Section 17 for Deposition and Section 22 for Particle Formation and Deposition)

80259. Martynenko, O.G., "Heat and Mass Transfer Bibliography: CIS Works," *Int. J. Heat Mass Transfer* 42, 197-217 (1999).

Heat/
Mass Transfer
CIS Works
Bibliography
520 References

80260. Viegas, D.X., "Forest Fire Propagation," *Phil. Trans. Roy. Soc. Lond. A* 356, 2907-2928 (1998).

Forest Fire
Propagation
Dynamics
Modeling

80261. Bishop, S.R., and D.D. Drysdale, "Fires in Compartments: The Phenomenon of Flashover," *Phil. Trans. Roy. Soc. Lond. A* 356, 2855-2872 (1998).

Compartment
Fire Spread
Flashover
Phenomenon
Modeling

(80089) Comparison with a Counterflow *n*-C_7H_{16}/Air Vapor Flame, Microprobe/Gas Chromatographic Species Profiles

Liquid Pool Flame

80262.	Wichman, I.S., "On Diffusion Flame Attachment Near Cold Surfaces," *Combust. Flame* 117, 384-393 (1999).	Flame/Surface Attachment Heat Losses Triple Flame Structure Modeling
80263.	Aghalayam, P., and D.G. Vlachos, "Roles of Thermal and Radical Quenching in Emissions of Wall-Stabilized Hydrogen Flames," *AIChE J.* 44, 2025-2034 (1998).	Gas/Surface H_2/Air Impinging Flame Radical Quenching NO,NO_2 Emissions Effects Modeling
(80184)	Turbulent Flowfield, Modifications, Modeling	Flame/Wall Interactions
(80143)	H_2/Air Ignition, Stability, Modeling	Wall Quenching Role
(80323)	Emissions Control, Conference Proceedings	Adsorbents Catalysts
(80346)	NO_x, SO_2 Control, Flue Gases, Review	Carbon Adsorbents
80264.	Chambrion, P., T. Kyotani and A. Tomita, "Role of N-Containing Surface Species on NO Reduction by Carbon," *Energy Fuels* 12, 416-421 (1998).	NO/Carbon Surface Reduction Mechanism Isotopic Labeling Measurements
80265.	Acke, F., and D. Stromberg, "Apparent Activation Energies for the Reduction of NO by CO and H_2 over Calcined Limestone and CaO Surfaces," *Energy Fuels* 12, 945-948 (1998).	NO/CO,H_2 CaO Surface Catalyzed Reduction Activation Energies
80266.	Ueda, A., T. Nakao, M. Azuma and T. Kobayashi, "Two Reaction Paths at Different Temperatures in the Reduction of Nitrogen Monoxide with Hydrogen over Supported Palladium Catalysts," *Chem. Lett. Jpn.* 595-596 (1998).	NO/H_2/O_2/Pt Catalytic Conversions N_2,N_2O Products T Effects
80267.	Schurath, U., and K.-H. Naumann, "Heterogeneous Processes Involving Atmospheric Particulate Matter," *Pure Appl. Chem.* 70, 1353-1361 (1998).	Heterogeneous Atmospheric Mechanisms Soot,NO_x,N_2O_5 Chemistry Overview

80268. Roberts, J.T., "Chemistry at the Surfaces of Ice and Sulfuric Acid: Toward an Understanding of Adsorption at Molecular Solids," *Acc. Chem. Res.* 31, 415-421 (1998).

Heterogeneous
Gas/Surface
Chemistry
Ice,H_2SO_4
Adsorption
Review

80269. Fickert, S., F. Helleis, J.W. Adams, G.K. Moortgat and J.N. Crowley, "Reactive Uptake of $ClNO_2$ on Aqueous Bromide Solutions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10689-10696 (1998).

Heterogeneous
$ClNO_2/H_2O$
$ClNO_2$/NaBr(aq)
$ClNO_2$/NaBr/NaCl(aq)
Uptake
Coefficients
Products
$ClNO_2$/He,N_2
Diffusion
Coefficients

80270. Chu, L.T., and L. Chu, "Studies of HBr Uptake on Ice Films at 188 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 384-395 (1999).

Heterogeneous
HBr/Ice
Uptake
Coefficients

80271. Chu, L., and L.T. Chu, "Heterogeneous Reaction $HOCl+HBr \rightarrow BrCl+H_2O$ on Ice Films," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 691-699 (1999).

Heterogeneous
HOCl/HBr(s)/Ice
Reaction
Probabilities
BrCl Formation

80272. Copeland, R.A., J.B. Pallix and D.A. Stewart, "Surface Catalyzed Production of NO from Recombination of N and O Atoms," *J. Thermophys. Heat Transfer* 12, 496-499 (1998).

Heterogeneous
N/O/Quartz
NO Formation
Room Temperature
LIF Measurements

(80340) Char Nitrogen, Kinetic Rates

Heterogeneous
N_2O Formation

80273. Cauquot, P., S. Cavadias and J. Amouroux, "Thermal Energy Accommodation from Oxygen Atoms Recombination on Metallic Surfaces," *J. Thermophys. Heat Transfer* 12, 206-213 (1998).

Heterogeneous
O/Metal
Accommodation
Coefficients
Cu,Ag,Co,Zn
Ni,Au,Steel

19. ENGINES/EMISSIONS

(See also Section 10 for Ignition)

80274. Yang, J., and R.W. Anderson, "A New Criterion for Judging Spark Ignition Engine In-Cylinder Pressure Development for Its Effect on Combustion Noise," *J. Eng. Gas Turb. Power, Trans. ASME* 120, 664-668 (1998).

I.C. Engine
In-Cylinder
Pressure
Combustion Noise
Relationships

80275. Ball, J.K., R.R. Raine and C.R. Stone, "Combustion Analysis and Cycle-by-Cycle Variations in Spark Ignition Engine Combustion. II. A New Parameter for Completeness of Combustion and Its Use in Modeling Cycle-by-Cycle Variations in Combustion," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 212, 507-523 (1998).

I.C. Engine
Cycle-to-Cycle
Variations
Combustion
Completeness
Pressure Monitoring
Parameter

80276. Golombok, M., P.J. Cooney, J.S. Kitching and S.R. Nattrass, "Spatial Resolution of Fuel Distribution in an Engine Using Infrared Absorption," *Rev. Sci. Instrum.* 68, 4236-4246 (1997).

I.C. Engine
Fuel Distribution
IR Absorption
Method

80277. Richter, M., B. Axelsson, K. Nyholm and M. Alden, "Real-Time Calibration of Planar Laser Induced Fluorescence Air/Fuel Ratio Measurements in Combustion Environments Using In Situ Raman Scattering," *Int. Symp. Combust.* 27, 51-57 (1998).

I.C. Engine
Fuel/Air
Ratio Monitor
Doped Fuel LIF
Raman Calibrator

80278. Sandrowitz, A.K., J.M. Cooke and N.G. Glumac, "Flame Emission Spectroscopy for Equivalence Ratio Monitoring," *Appl. Spectrosc.* 52, 658-662 (1998).

Equivalence Ratio
Flame Monitor
CH,OH
Spectral Emission
CH_4/Air
C_2H_2/O_2

80279. Arcoumanis, C., M.R. Gold, J.H. Whitelaw and H.M. Xu, "Local Mixture Injection to Extend the Lean Limit of Spark Ignition Engines," *Experiments Fluids* 26, 126-135 (1999).

I.C. Engines
Lean C_3H_8/Air
Spark Plug Region
Trace Injection
Performance

80280. Kaminski, C.F., J. Engstrom and M. Alden, "Quasi-Instantaneous Two-Dimensional Temperature Measurements in a Spark Ignition Engine Using 2-Line Atomic Fluorescence," *Int. Symp. Combust.* 27, 85-93 (1998).

I.C. Engine
2-D Temperatures
Indium 2-Line
Fluorescence
Method

80281. Jenkin, R.J., E.H. James and W.M. Malalasekera, "Modeling the Effects of Combustion and Turbulence on Near-Wall Temperature Gradients in the Cylinders of Spark Ignition Engines," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 212, 533-546 (1998).

I.C. Engines
Near Wall
T Gradients
Turbulence
Model

80282. Min, K., and W.K. Cheng, "Oil Layer as Source of Hydrocarbon Emissions in Spark Ignition Engines," *J. Eng. Gas Turb. Power, Trans. ASME* 120, 669-677 (1998).

I.C. Engines
UHC Emissions
Liner Oil Layer
Source
Model

80283. Parks II, J.E., J.S. Armfield, T.E. Barber, J.M.E. Storey and E.A. Wachter, "In Situ Measurement of Fuel in the Cylinder Wall Oil Film of a Combustion Engine by LIF Spectroscopy," *Appl. Spectrosc.* 52, 112-118 (1998).

I.C. Engines
Unburnt
Hydrocarbons
Cylinder Wall
Oil Film
LIF Monitor

80284. Huang, Z., J. Pang, K. Pan, D. Jiang, L. Zhou and Z. Yang, "Investigation into Hydrocarbon Emissions from Crevice and Oil Film During Cold Start and Idling Periods in a Spark Ignition Engine," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 212, 501-505 (1998).

I.C. Engine
Crevice,Liner
UHC Emissions
Cold,Idle
Conditions

(80469) Photoionization/Mass Analysis, Automobile Exhaust Monitor

Aromatic Emissions

80285. Jingding, L., G. Linsong and D. Tianshen, "Formation and Restraint of Toxic Emissions in Hydrogen/Gasoline Mixture Fueled Engines," *Int. J. Hydrogen Energy* 23, 971-975 (1998).

I.C. Engines
Gasoline/H_2
NO_x Emissions
Effects

80286. Yacoub, Y., R. Bata and M. Gautam, "The Performance and Emission Characteristics of C_1-C_5 Alcohol/Gasoline Blends with Matched Oxygen Content in a Single-Cylindrical Spark Ignition Engine," *Proc. Inst. Mech. Eng. A. J. Power Energy* 212, 363-379 (1998).

I.C. Engine
C_1-C_5 Alcohol/
Gasoline Blends
UHC,CO,NO
ROH,RCHO
Emissions

80287. Gouli, S., E., Lois and S. Stournas, "Effects of Some Oxygenated Substitutes on Gasoline Properties, Spark Ignition Engine Performance and Emissions," *Energy Fuels* 12, 918-924 (1998).

I.C. Engines
Furan Derivatives
p-Cresol
Additives
Ignition Effects
HC,CO,NO_x
Emissions

80288. Pischinger, F.F., "The Diesel Engine for Cars: Is There a Future?," *J. Eng. Gas Turb. Power, Trans. ASME* 120, 641-647 (1998).

Diesel Engines
Passenger Car
Increased Market
Development
Problems

80289. Salem, H., S.H. El-Bahnasy and M. Elbaz, "Prediction of the Effect of Injection Parameters on NO_x Emission and Burning Quality in the Direct Injection Diesel Engine Using a Modified Multizone Model," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 212, 427-436 (1998).

Diesel Engine
Multispray Injectors
2-Zone Cylinder
Performance
NO_x Formation
Modeling

80290. Karonis, D., E. Lois, S. Stournas and F. Zannikos, "Correlations of Exhaust Emissions from a Diesel Engine with Diesel Fuel Properties," *Energy Fuels* 12, 230-238 (1998).

Diesel Engine
Fuel/Emissions
Correlations
UHC,CO
NO,Soot

80291. Ergeneman, M., C. Sorusbay and A.G. Goktan, "Exhaust Emission and Fuel Consumption of CNG/Diesel Fueled City Buses Calculated Using a Sample Driving Cycle," *Energy Sources* 21, 257-268 (1999).

Diesel Engines
Dual Fuel
CNG/Diesel
CO,NO_x
Particle Emissions

80292. Sato, Y., T. Sakamoto and A. Noda, "Major Factors of EGR on Improvement in NO_x and Thermal Efficiency in a Direct-Injection Methanol Engine," *JSAE Review* 14(4), 62-64 (1993).

Diesel Engine
CH_3OH
EGR Effects
Performance
NO_x Emissions

80293. Ladommatos, N., S.M. Abdelhalim, H. Zhao and Z. Hu, "The Effects of Carbon Dioxide in Exhaust Gas Recirculation on Diesel Engine Emissions," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 212, 25-42 (1998).

Diesel Engines
EGR
CO_2 Additives
Performance
NO_x ,Particulate
Effects

80294. Ladommatos, N., S.M. Abdelhalim and H. Zhao, "Effects of Exhaust Gas Recirculation Temperature on Diesel Engine Combustion and Emissions," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 212, 479-500 (1998).

Diesel Engines
EGR
UHC,NO_x ,Soot
Emissions
Effects

80295. Murayama, T., T. Chikahisa and Y. Fujiwara, "Diesel Engine Smoke Reduction by Controlling Early Thermal Cracking Process and Activation Later Stage Combustion," *J. Eng. Gas Turb. Power, Trans. ASME* 120, 648-656 (1998).

Diesel Engine
Soot Control
Oxygenated
Fuel Addition
Turbulence
Enhancements
NO Effects

80296. Vattulainen, J., R. Hernberg, C. Hattar and S. Gros, "Fast Exhaust Channel Optical Absorption Method and Apparatus to Study the Gas Exchange in Large Diesel Engines," *Rev. Sci. Instrum.* 69, 277-285 (1998).

Diesel Engine
SO_2
Absorption
Exhaust Gases
Measurements

20. PLUME/STACK CHEMISTRY/ATMOSPHERIC EMISSIONS

(See also Section 18 for Gas/Surface Uptake Coefficients and Section 30 for Atmospheric Monitoring Methods)

80297.	Craig, K.J., D.J. De Kock and J.A. Snyman, "Using CFD and Mathematical Optimization to Investigate Air Pollution Due to Stacks," *Int. J. Numer. Methods Eng.* 44, 551-565 (1999).	Stack Dispersal CFD Model
(80267)	Atmospheric Chemistry, Soot, NO_x, N_2O_5, Overview	Heterogeneous Mechanisms
80298.	Atkinson, R., "Product Studies of Gas Phase Reactions of Organic Compounds," *Pure Appl. Chem.* 70, 1335-1343 (1998).	Atmospheric Organics Degradation Chemistry Product Studies
80299.	Atkinson, R., "Gas Phase Degradation of Organic Compounds in the Troposphere," *Pure Appl. Chem.* 70, 1327-1334 (1998).	Tropospheric Organics Degradation Chemistry Overview
80300.	Atkinson, R., and J. Arey, "Atmospheric Chemistry of Biogenic Organic Compounds," *Acc. Chem. Res.* 31, 574-583 (1998).	Atmospheric Bio-Organics OH, O_3, NO Reactions Products Lifetimes
80301.	Crutzen, P.J., "How the Atmosphere Keeps Itself Clean and How This is Affected by Human Activities," *Pure Appl. Chem.* 70, 1319-1326 (1998).	Atmospheric Chemistry CH_4, NO, O_3 Budgets Anthropogenic Effects
80302.	Semiletov, I.P., "Aquatic Sources and Sinks of CO_2 and CH_4 in the Polar Regions," *J. Atmos. Sci.* 56, 286-306 (1999).	Atmospheric CH_4, CO_2 Aquatic Polar Sources/Sinks
80303.	Reichle Jr, H.G., and V.S. Connors, "The Mass of CO in the Atmosphere During October 1984, April 1994 and October 1994," *J. Atmos. Sci.* 56, 307-310 (1999).	Atmospheric CO Increases
80304.	Wang, J., J.C. Gille, P.L. Bailey, L. Pan, D. Edwards and J.R. Drummond, "Retrieval of Tropospheric Carbon Monoxide Profiles from High Resolution Interferometer Observations: A New Digital Gas Correlation Method and Applications," *J. Atmos. Sci.* 56, 219-232 (1999).	Tropospheric CO Profiles Interferometric Global Measurements

80305. Shirai, T., and Y. Makide, "Rapidly Increasing Concentrations of CFC Alternatives (HFC-134a, HCFC-141b, and HCFC-142b) in the Atmosphere as Observed in Hokkaido and Antarctica," *Chem. Lett. Jpn.* 357-358 (1998).

Atmospheric
CH_2FCF_3
CH_3CClF_2
CH_3CCl_2F
Concentrations
Trends

80306. Waters, J.W., W.G. Read, L. Froidevaux, R.F. Jarnot, R.E. Cofield, D.A. Flower, G.K. Lau, H.M. Pickett, M.L. Santee, D.L. Wu, M.A. Boyles, J.R. Burke, R.R. Lay, M.S. Loo, N.J. Livesey, T.A. Lungu, G.L. Manney, L.L. Nakamura, V.S. Perun, B.P. Ridenoure, Z. Shippony, P.H. Siegel, R.P. Thurstans, R.S. Harwood, H.C. Pumphrey and M.J. Filipiak, "The Upper Atmosphere Research Satellite and Earth Observing System Microwave Limb Sounder Experiments," *J. Atmos. Sci.* 56, 194-218 (1999).

Stratospheric
ClO,H_2O,O_3
Microwave
Emission
Satellite
Measurements

(80404) Atmospheric Infrared Measurements, Spectroscopic Applications, Overview

$ClONO_2,HNO_3$

80307. Mosier, A.R., J.M. Duxbury, J.R. Freney, O. Heinemeyer and K. Minami, "Assessing and Mitigating N_2O Emissions from Agricultural Soils," *Climatic Change* 40, 7-38 (1998).

Atmospheric
N_2O
Agricultural
Source Strengths

80308. Evans, W.F.J., and E. Puckrin, "Remote Sensing Measurements of Tropospheric Ozone by Ground Based Thermal Emission Spectroscopy," *J. Atmos. Sci.* 56, 311-318 (1999).

Tropospheric
O_3
FTIR Thermal
Emission Monitor

80309. Burrows, J.P., M. Weber, M. Buchwitz, V. Rozanov, A. Ladstatter-Weissenmayer, A. Richter, R. DeBeek, R. Hoogen, K. Bramstedt, K.-U. Eichmann, M. Eisinger and D. Perner, "The Global Ozone Monitoring Experiment: Mission Concept and First Scientific Results," *J. Atmos. Sci.* 56, 151-175 (1999).

Atmospheric
O_3,BrO,ClO_2
$SO_2,HCHO$
Global
Satellite
Measurements

80310. Hansen, J., M. Sato, J. Glascoe and R. Ruedy, "A Common-Sense Climate Index: Is Climate Changing Noticeably?," *Proc. Nat. Acad. Sci. USA* 95, 4113-4120 (1998).

Climatic Impact
Change Index
Assessment

80311. Jones, P.D., R.S. Bradley and J. Jouzel, eds., *"Climatic Variations and Forcing Mechanisms of the Last 2000 Years,"* 30 Papers Presented at a Workshop Held in Il Ciocco, Lucca, Italy, October 1994, *NATO Adv. Study Instit. Ser. I. Global Environ. Change* 41, 649 pp. (1996).

Climatic Impact
Forcing
Mechanisms
Workshop
Proceedings

80312. Ramstein, G., Y. Serafini-Le Treut, H. Le Treut, M. Forichon and S. Joussaume, "Cloud Processes Associated with Past and Future Climate Changes," *Climate Dyn.* 14, 233-247 (1998).

Climatic Impact
Cloud Feedback
Dynamics

80313.	Mosier, A.R., J.M. Duxbury, J.R. Freney, O. Heinemeyer, K. Minami and D.E. Johnson, "Mitigating Agricultural Emissions of Methane," *Climatic Change* 40, 39-80 (1998).	Climatic Impact CH_4 Mitigating Agricultural Emissions Methods
80314.	Cai, W., and H.B. Gordon, "Transient Responses of the CSIRO Climate Model to Two Different Rates of CO_2 Increase," *Climate Dyn.* 14, 503-516 (1998).	Climatic Impact CO_2 Rate of Increase Warming Scenarios Modeling
80315.	Rind, D., D. Shindell, P. Lonergan and N.K. Balachandran, "Climate Change and the Middle Atmosphere. III. The Doubled CO_2 Climate Revisited," *J. Climate* 11, 876-894 (1998).	Climatic Impact CO_2 Tropospheric/ Stratospheric Responses
80316.	Shindell, D.T., D. Rind and Patrick Lonergan, "Climate Change and the Middle Atmosphere. IV. Ozone Response to Doubled CO_2," *J. Climate* 11, 895-918 (1998).	Climatic Impact CO_2 Effects on O_3 Photochemical Model
80317.	Wigley, T.M.L., P.J. Jaumann, B.D. Santer and K.E. Taylor, "Relative Detectability of Greenhouse Gas and Aerosol Climate Change Signals," *Climate Dyn.* 14, 781-790 (1998).	Climatic Impact CO_2,Aerosols Change Detectability Difficulties
80318.	Le Treut, H., M. Forichon, O. Boucher and Z.-X. Li, "Sulfate Aerosol Indirect Effect and CO_2 Greenhouse Forcing: Equilibrium Response of the Laboratoire de Meteorologie Dynamique GCM and Associated Cloud Feedbacks," *J. Climate* 11, 1673-1684 (1998).	Climatic Impact CO_2,SO_4^{2-} Radiative Forcing Sensitivities
80319.	Reader, M.C., and G.J. Boer, "The Modification of Greenhouse Gas Warming by the Direct Effect of Sulfate Aerosols," *Climate Dyn.* 14, 593-607 (1998).	Climatic Impact CO_2,SO_4^{2-} Offset Effects Modeling
80320.	Chen, Y.-j., H. Zhang and X. Bi, "Numerical Experiment for the Impact of the Ozone Hole over Antarctica on the Global Climate," *Adv. Atm. Sci.* 15, 300-311 (1998).	Climatic Impact Ozone Hole Global Effects Modeling
80321.	Qian, Y., H. Wang, C. Fu and Z.-f. Wang, "Seasonal and Spatial Variation of Radiative Effects of Anthropogenic Sulfate Aerosol," *Adv. Atm. Sci.* 15, 380-392 (1998).	Climatic Impact SO_4^{2-} Aerosols Seasonal Spatial Variations

80322. Penner, J.E., C.C. Chuang and K. Grant, "Climate Forcing by Carbonaceous and Sulfate Aerosols," *Climate Dyn.* 14, 839-851 (1998).

Climatic Impact
SO_4^{2-},Soot
Atmospheric Aerosols
Radiative
Forcing Effects

21. COMBUSTION EMISSIONS/NO_X, SO_2 CHEMISTRY, CONTROL

(See also Section 19 for Engine Emissions)

80323. Lu, G.Q., and V. Rudolph, eds., "Adsorbents and Catalysts for Clean Energy and Emissions Control," Special Issue, 13 Papers Presented at the *2nd Asia Pacific Conference on Sustainable Energy and Environmental Technology*, Held in Gold Coast, Australia, June 1998, *Energy Fuels* 12, 1049-1141 (1998).

Emissions Control
Adsorbents
Catalysts
Conference
Proceedings

80324. Griffin, P.G., R.J.S. Morrison, A. Campisi and B.L. Chadwick, "Apparatus for the Detection and Removal of Vapor Phase Alkali Species from Coal Derived Gases at High Temperature and Pressure," *Rev. Sci. Instrum.* 69, 3674-3677 (1998).

Alkali Emissions
Absorption Control
Alumino-Silicate
Clays
Photofragment
Fluorescence
Monitoring

80325. Korzekwa, R.A., M.G. Grothaus, R.K. Hutcherson, R.A. Roush and R. Brown, "Destruction of Hazardous Air Pollutants Using a Fast Rise Time Pulsed Corona Reactor," *Rev. Sci. Instrum.* 69, 1886-1892 (1998).

Incineration
CF_2Cl_2,CH_2Cl_2
$C_6H_5CH_3$
Pulsed Discharge
Method

80326. Kim, H.J., C.H. Cho, H. Kim and S.C. Lee, "Decomposition of Carbon Tetrachloride in Air Plasma Using Glow Discharge Atomic Emission Spectrometry," *Analyst* 123, 607-610 (1998).

Discharge
Incineration
CCl_4/Air
Cl,Cl_2 Spectral
Emission

80327. Hsieh, L.-T., W.-J. Lee, C.-Y. Chen, Y.-P.G. Wu, S.-J. Chen and Y.-F. Wang, "Decomposition of Methyl Chloride by Using a Radiofrequency Plasma Reactor," *J. Hazardous Mat. B* 63, 69-90 (1998).

Incineration
RF Plasma Reactor
CH_3Cl/O_2
Products
Efficiencies

(80113) Zeolites, C_6H_5Cl/Air Oxidation, Waste Disposal

Catalytic
Incineration

(80112) Foam Ceramic Burner, CH_4/Air, Destruction of VOCs

Catalytic
Incineration

80328.	Hilton, M., A.H. Lettington and C.W. Wilson, "Gas Turbine Exhaust Emissions Monitoring Using Nonintrusive Infrared Spectroscopy," Presented Originally as Paper 97-GT-180 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 514-518 (1998).	Gas Turbine Exhausts FTIR Emission T,CO,CO_2 Monitoring
(80524)	C_2H_4/O_2 Flames, Formation Mechanisms, Kinetic Modeling Simulation	Aromatics,PAHs
(80472)	Incinerator, On-line Flue Gases Monitor, REMPI/TOFMS Method	$C_{10}H_8$,PAHs
80329.	Revuelta, C.C., E.de la F. Santiago and J.A.R. Vazquez, "Characterization of Polycyclic Aromatic Hydrocarbons in Emissions from Coal Fired Power Plants: The Influence of Operation Parameters," *Environ. Technol.* 20, 61-68 (1999).	PAH Emission Coal Combustion 5 Power Plants
80330.	Kotler, V.R., "The Problem of NO_x Emissions from Coal Fired Electric Power Stations in the United States," *Thermal Eng., Russia* 45, 253-259 (1998).	NO_x Emissions Coal Fired Electric Utilities US Assessments
80331.	Feitelberg, A.S., and M.A. Lacey, "The GE Rich-Quench-Lean Gas Turbine Combustor," Presented Originally as Paper 97-GT-127 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 502-508 (1998).	Low NO_x ,CO Turbine Combustor Rich/Lean Design
(80114)	Catalytic Combustor, Gas Turbine Application	Low NO_x Emissions
80332.	Hasegawa, T., M. Sato and T. Ninomiya, "Effect of Pressure on Emission Characteristics in Low Btu Gas-Fueled 1500°C-Class Gas Turbine," Presented Originally as Paper 97-GT-277 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 481-487 (1998).	NO_x Emissions Low Btu Gas Fueled Gas Turbine Performance Testing
80333.	Tonouchi, J.H., T.J. Held and H.C. Mongia, "A Semi-Analytical Finite Rate Two-Reactor Model for Gas Turbine Combustors," Presented Originally as Paper 97-GT-126 at the *42nd International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Orlando FL, June 1997, *J. Eng. Gas Turbines, Trans ASME* 120, 495-501 (1998).	NO_x ,CO Emissions Gas Turbine Mixing/Kinetic Model
80334.	Nakata, T., M. Sato and T. Hasegawa, "Reaction of Fuel NO_x Formation for Gas Turbine Conditions," Presented Originally at the *4th ASME/JSME Thermal Engineering Joint Conference*, Held in Maui, HI, March 1995, *J. Eng. Gas Turb. Power, Trans. ASME* 120, 474-480 (1998).	NO_x Formation Fuel 'N' Gas Turbines Kinetic Modeling
(80077)	Char 'N', Combustion, Structural Dependences	NO_x Formation
80335.	Coda, B., F. Kluger, D. Fortsch, H. Spliethoff, K.R.G. Hein and L. Tognotti, "Coal-Nitrogen Release and NO_x Evolution in Air-Staged Combustion," *Energy Fuels* 12, 1322-1327 (1998).	NO_x Formation Coal Combustion Reactor Air Staging Nitrogen Fate Measurements

80336.	Steele, R.C., J.H. Tonouchi, D.G. Nicol, D.C. Horning, P.C. Malte and D.T. Pratt, "Characterization of NO_x, N_2O and CO for Lean-Premixed Combustion in a High Pressure Jet-Stirred Reactor," Presented Originally as Paper 96-GT-128 at the *41st International Gas Turbine and Aeroengine Congress and Exhibition*, Held in Birmingham UK, June 1996, *J. Eng. Gas Turbines, Trans. ASME* 120, 303-310 (1998).	NO_x ,N_2O Formation CO Oxidation Lean Premixed Jet Stirred Reactor Measurements
80337.	Gasnot, L., P. Desgroux, J.F. Pauwels and L.R. Sochet, "Detailed Analysis of Low-Pressure Premixed Flames of $CH_4+O_2+N_2$: A Study of Prompt NO," *Combust. Flame* 117, 291-306 (1999).	Prompt NO Formation $CH_4/O_2/N_2$ T,Species LIF,GC Monitoring Kinetic Model Adequacies
(80195)	CH_4 /Air Turbulent Combustion, Gas Turbines, Kinetic Modeling, Reduced Schemes	NO_x Formation
(80196)	Turbulent H_2/O_2/He, Kinetic/Radiative Submodels	NO Formation
(80263)	H_2 /Air, Gas/Surface Impinging Flame, Radical Quenching, Numerical Modeling	NO,NO_2 Emissions
80338.	Bourdon, A., A. Leroux, P. Domingo and P. Vervisch, "Experiment-Modeling Comparison in a Nonequilibrium Supersonic Air Nozzle Flow," *J. Thermophys. Heat Transfer* 13, 68-75 (1999).	NO Formation Supersonic Air Nozzle Flow Nonequilibrium Relaxation Effects
80339.	Bose, D., and G.V. Candler, "Advanced Model of Nitric Oxide Formation in Hypersonic Flows," *J. Thermophys. Heat Transfer* 12, 214-222 (1998).	NO Formation Hypersonic Flows Zeldovich Mechanism Nonequilibrium Effects
80340.	De Soete, G.G., E. Croiset and J.-R. Richard, "Heterogeneous Formation of Nitrous Oxide from Char-Bound Nitrogen," *Combust. Flame* 117, 140-154 (1999).	N_2O Formation Heterogeneous Char Nitrogen Kinetic Rates
80341.	Gritsenko, E.A., V.N. Orlov, A.M. Postnikov and Yu.I. Tsybizov, "Reducing NO_x Emissions when Converting Aircraft Engines," *Thermal Eng., Russia* 45, 240-245 (1998).	NO_x Control Aircraft Engines Retrofitting Technologies
(80188)	Reciprocal Vortex Stabilized Flame, Enhanced Thermal Efficiencies	NO_x Control

80342. Yuan, J., and I. Naruse, "Effects of Air Dilution on Highly Preheated Air Combustion in a Regenerative Furnace," *Energy Fuels* 13, 99-104 (1999).

NO_x Control
Highly Preheated Air Combustion
CO_2 ,N_2 ,He,Ar
Flue Gas Dilution Effects

80343. Alzueta, M.U., R. Bilbao, A. Millera, P. Glarborg, M. Ostberg and K. Dam-Johansen, "Modeling Low Temperature Gas Reburning: NO_x Reduction Potential and Effects of Mixing," *Energy Fuels* 12, 329-338 (1998).

NO_x Control
Reburn Method
C_1 ,C_2 Hydrocarbons
Mixing/Kinetic Model

80344. Xu, H., L.D. Smoot and S.C. Hill, "A Reduced Kinetic Model for NO_x Reduction by Advanced Reburning," *Energy Fuels* 12, 1278-1289 (1998).

NO_x Control
Reburn Method
CH_4 /NH_3
Full/Reduced Kinetic Models

80345. Nakagawa, Y., and H. Kawauchi, "Pulse Intense Electron Beam Irradiation on the Atmospheric Pressure N_2 Containing 220 ppm of NO," *Jpn. J. Appl. Phys.* 37, 5082-5087 (1998).

NO Control
e^--Beam Method
Efficiencies

80346. Omel'chenko, Yu.M., A.I. Blokhin, A.N. Nikitin, S.Yu. Shan'ko and V.V. Lutchina, "Using Carbon Adsorbents for Removing Nitrogen Oxides and Sulfur Oxides from the Flue Gases," *Thermal Eng., Russia* 45, 970-973 (1998).

NO_x ,SO_2 Control
Flue Gases
Carbon Adsorbents
Review

80347. Amirov, R.H., J.O. Chae, Y.N. Dessiaterik, E.A. Filimonova and M.B. Zhelezniak, "Removal of NO_x and SO_2 from Air Excited by Streamer Corona: Experimental Results and Modeling," *Jpn. J. Appl. Phys.* 37, 3521-3529 (1998).

NO_x ,SO_2 Control
Corona Discharge Method
NH_3 Addition
Efficiencies

22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Soot Formation in Engines)

80348. Brown, A.L., and T.H. Fletcher, "Modeling Soot Derived from Pulverized Coal," *Energy Fuels* 12, 745-757 (1998).

Soot Formation
Pulverized Coal
Semiempirical
Combustion Model
Transport/
Radiative Properties

80349. Smooke, M.D., C.S. McEnally, L.D. Pfefferle, R.J. Hall, and M.B. Colket, "Computational and Experimental Study of Soot Formation in a Coflow, Laminar Diffusion Flame," *Combust. Flame* 117, 117-139 (1999).

Soot Formation
Growth
CH_4 /Air
Modeling Adequacies

(80093)	Microgravity Combustion of Fuel Droplets, n-C_7H_{16}, n-C_9H_{20}, Visualizations	Soot Shell Structures
80350.	Tait, N.P., "Soot Formation in Cracked Flames," *Combust. Flame* 117, 435-437 (1999).	Soot Formation i-C_8H_{18}/Air Flame Surface Inhomogeneity Effects
80351.	Vander Wal, R.L., "Calibration and Comparison of Laser Induced Incandescence with Cavity Ringdown," *Int. Symp. Combust.* 27, 59-67 (1998).	Soot Volume Fractions LII Monitor Cavity Ringdown Calibration
(80116) (80117)	Catalytic Combustion	Soot Oxidation
80352.	Piekarczyk, W., "How and Why CVD Diamond is Formed: A Solution of the Thermodynamic Paradox," *J. Mater. Sci.* 33, 3443-3453 (1998).	Diamond Formation CVD Methods Thermodynamic Enigma Resolution
80353.	Shima-Edelstein, R., I. Gouzman and A. Hoffman, "Nucleation and Initial Growth Stages of Chemical Vapor Deposition (CVD) Diamond," *Isr. J. Chem.* 38, 17-31 (1998).	Diamond Formation Nucleation Initial Growth Incubation Times Substrate Pretreatment
80354.	Kim, J.S., and M.A. Cappelli, "Competing Surface Oxidation Reactions During Diamond Synthesis in Low Pressure Flames," *Jpn. J. Appl. Phys.* 37, 6223-6228 (1998).	Diamond Formation CH_4,C_2H_4,C_2H_2/O_2 Flames Surface Oxidation Growth Rate Model Adequacies
80355.	Rozbicki, R.T., and V.K. Sarin, "Nucleation and Growth of Combustion Flame Deposited Diamond on Silicon Nitride," *Int. J. Refractory Hard Metals* 16, 377-388 (1998).	Diamond Formation C_2H_2/O_2 Flame Si_3N_4 Substrate Temperature Effects Activation Energies
80356.	Yu, J., R. Huang, L. Wen and C. Shi, "Effects of Density of Gas Flow Rate on Large Area Diamond Growth in Hot Filament Chemical Vapor Deposition," *J. Mater. Sci. Lett.* 17, 1011-1013 (1998).	Diamond Formation Heated Filament Large Area Growth Flow Rate Density Effects

80357. Werner, M., and R. Locher, "Growth and Application of Undoped and Doped Diamond Films," *Rpts. Prog. Phys.* 61, 1665-1710 (1998).

Diamond Formation
Heated Filament
Microwave Methods
Growth,Doping
Properties
Applications
Review

80358. Brunsteiner, R., R. Haubner and B. Lux, "Influence of Carbon Monoxide Addition to the Reaction Gas on the Hot Filament Diamond Deposition," *Int. J. Refractory Hard Metals* 14, 127-135 (1996).

Diamond Formation
CH_4/H_2
Heated Filament
CO Addition
Effects
Growth Rates

80359. Kalss, W., S. Bohr, R. Haubner, B. Lux, M. Griesser, H. Spicka, M. Grasserbauer and P. Wurzinger, "Influence of Boron on Diamond Growth on WC-Co Hardmetals," *Int. J. Refractory Hard Metals* 14, 137-144 (1996).

Diamond Formation
Heated Filament
$B(C_2H_5)_3$ Effects
Differing
Substrates

80360. Girshick, S.L., and J.M. Larson, "Thermal Plasma Synthesis of Diamond," *Pure Appl. Chem.* 70, 485-492 (1998).

Diamond Formation
RF Discharge Method
Surface Sampling
GC Analysis
Species Densities

80361. Laimer, J., W. Putz, H. Stori, P. Janz and H. Winkler, "Growth of Diamond in an Electrodeless Capacitive Radiofrequency Discharge," *Int. J. Refractory Hard Metals* 14, 173-178 (1996).

Diamond Formation
$CH_4/CO_2/H_2$
RF Discharge
SiC Substrate
Growth Morphologies

80362. Haubner, R., A. Lindlbauer and B. Lux, "Diamond Nucleation and Growth on Refractory Metals Using Microwave Plasma Deposition," *Int. J. Refractory Hard Metals* 14, 119-125 (1996).

Diamond Formation
Microwave Discharge
Method
Refractory Metal
Substrate
Pretreatments

80363. Farhat, S., C. Findeling, F. Silva, K. Hassouni and A. Gicquel, "Role of the Plasma Composition at the Surface on Diamond Growth," *J. de Phys. IV. Colloque* 8(7), 391-399 (1998).

Diamond Formation
Microwave Discharge
Plasma/Surface
Composition
Model
H-Atom Monitoring

80364. Laimer, J., and S. Matsumoto, "Pulsed Microwave Plasma-Assisted Chemical Vapor Deposition of Diamond," *Int. J. Refractory Hard Metals* 14, 179-184 (1996).

Diamond Formation
$CH_4/H_2/Ar$
Microwave Discharge
H Atom/
Growth Rates

80365. Zhang, H.-X., Z. Lin, Y.-B. Jiang, K.-A. Feng and S.-Z. Yang, "Diamond Nucleation Using a Pulsed High Temperature and High-Density CH_4 Plasma Beam," *J. Mater. Sci. Lett.* 17, 1515-1518 (1998).

Diamond Formation
CH_4
Plasma Beam
Enhanced Nucleation

80366. Kawasaki, H., K. Sakamoto, S. Maeda, T. Fukuzawa, M. Shiratani and Y. Watanabe, "Study on Initial Growth of Particles in Low Pressure and Low-Power GeH_4 Radiofrequency Discharges Using the High-Sensitivity Photon Counting Laser Light Scattering Method," *Jpn. J. Appl. Phys. Lett. B* 37, L1264-L1267 (1998).

Particle Formation
Growth
GeH_4/Ar
Discharge
GeH_2 Role

80367. Kawasaki, H., K. Sakamoto, S. Maeda, T. Fukuzawa, M. Shiratani and Y. Watanabe, "Transition of Particle Growth Region in SiH_4 Radiofrequency Discharges," *Jpn. J. Appl. Phys.* 37, 5757-5762 (1998).

Particle Formation
Growth Rate
SiH_4 Discharge
Parameter Dependences

23. PARTICLE CHARACTERIZATION

(See also Section 5 for Spray Characterization)

80368. Chan, C.C.Y., and D.W. Kirk, "Behavior of Metals under the Conditions of Roasting Municipal Solid Waste Incinerator Fly Ash with Chlorinating Agents," *J. Hazardous Mat.B* 64, 75-89 (1999).

Fly Ash
Incinerator
Sample Analysis
32 Trace Elements
Cl Volatilization
Efficiencies

80369. Damaschke, N., G. Gouesbet, G. Grehan and C. Tropea, "Optical Techniques for the Characterization of Non-Spherical and Non-Homogeneous Particles," *Measurement Sci. Technol.* 9, 137-140 (1998).

Particles
Non-spherical
Nonhomogeneous
Characterizations
Optical Methods
Review

24. NUCLEATION/COAGULATION/CLUSTERS

(See also Section 22 for Nucleation and Growth of Particles)

(80759) Structural Calculations, Geometries, Binding Energies — $Ag^+(H_2O)_n$, $Au^+(H_2O)_n$ $Cu^+(H_2O)_n$, n=1-4

(80832) Photoelectron Spectra, Constants, S/O Splitting, $D_0(As_n^-)$, EA(As_n) — As_n^-, n=1-5

(80436) Predissociation, v=10, 39-48, Product Br_2(B,v,J) Distributions, Measurements — Br_2(B).He

(80393) Millimeter Wave Transitions, Measurements — $(CO)_2$

(80386) FTIR Spectra, Frequencies, Matrix Study — $(CO_2)_2^-$, CO_2^-

80370. Van Orden, A., and R.J. Saykally, "Small Carbon Clusters: Spectroscopy, Structure and Energetics," *Chem. Rev.* 98, 2313-2357 (1998).

C_n ,$C_n^{\pm}$
Spectroscopy
Structure
Energies
Review

80371. Satishkumar, B.C., A. Govindaraj, R. Sen and C.N.R. Rao, "Single-Walled Nanotubes by the Pyrolysis of Acetylene-Organometallic Mixtures," *Chem. Phys. Lett.* 293, 47-52 (1998).

C_n Nanotubes
$C_2H_2/Fe(CO)_5/Ar$
Pyrolysis
Formation

(80400) Infrared Absorption, Cavity Ringdown Spectrum

$C_{60}(s)$

80372. Dauw, X.L.R., M.V. Bronsveld, A. Kruger, J.B.M. Warntjes, M.R. Witjes and E.J.J. Groenen, "On the Singlet Excited States of C_{70} and C_{60}" *J. Chem. Phys.* 109, 9332-9339 (1998).

C_{60} ,C_{70}
Solutions
Phosphorescent
Spectra
Excited States

(80586) (80587) Photofragment Mass Spectra, Anomalies, Cluster Effects

C_{60}

(80245) Ionization Cross Sections, Product Ions

$C_{60}+e^-$

(80858) Thermodynamic Values, fef, S°, H_T-H_0, ΔH_f, ΔG_f, ΔS_f, Measurements

$C_{70}(s)$

(80588) Product ClO, O Energies, Cluster Effects

$(ClO_2)_n+h\nu$
$ClO_2Ar_n+h\nu$
$ClO_2(H_2O)_n+h\nu$

(80441) Predissociation Lifetimes, Product States, Calculations

$Cl_2(B,v).Ne$

80373. Paul, J.B., R.A. Provencal, C. Chapo, A. Petterson and R.J. Saykally, "Infrared Cavity Ringdown Spectroscopy of Water Clusters: O-D Stretching Bands," *J. Chem. Phys.* 109, 10201-10206 (1998).

$(D_2O)_n$
$n=2$-8
IR ν_{OD} Spectra
Assignments
Cavity Ringdown

80374. Hossenlopp, J.M., D.T. Anderson, M.W. Todd and M.I. Lester, "State-to-State Inelastic Scattering from Vibrationally Activated OH-H_2 Complexes," *J. Chem. Phys.* 109, 10707-10718 (1998).

$H_2.OH(2\nu_{OH})$
Half Collision
Predissociation
Reaction
OH(v=1,J) Product
IR Pump/UV Probe

(80744) P.E. Surface, Photodissociation, Dynamics, Calculations

$H_2O(A).Ar_n$

(80446) fs Pump/Probe Dissociating State Motion

$I_2(B).Rg$

(80593) Dynamics, Calculations, Theoretical Difficulties

$Na.HF+h\nu$

(80873) Geometries, Frequencies, Dissociation Energies, Measurements, Calculations

$Ni^+(H_2)_n$,n=1-6

(80426) LIF Spectra, Constants, P.E. Surfaces — OH.Kr(A-X) OD.Kr(A-X)

(80754) P.E. Curves, DIM Calculation Method — SH.Kr (A,X)

(80876) Geometries, DFT Calculations, n=2-9 — $D(V_n, V_n^+)$ $IP(V_n)$

80375. Holmgren, L., and A. Rosen, "Vanadium Clusters: Reactivity with CO, NO, O_2, D_2 and N_2," *J. Chem. Phys.* 110, 2629-2636 (1999). — $V_n + CO, D_2$ $V_n + NO, N_2, O_2$ n=10-60 Reaction Probabilities

25. FLAME/CHEMILUMINESCENT SPECTROSCOPY

26. SPECTRAL CHARACTERIZATIONS/ANALYSES

(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

80376. Omenetto, N., J.-M. Mermet, G.C. Turk and D.S. Moore, "Laser Based Atomic Spectroscopy: A New Notation for Spectrochemical Processes, IUPAC Recommendations 1997," *Pure Appl. Chem.* 70, 517-526 (1998). — Laser Atomic Spectroscopy LIF, MPI Nomenclature Recommendations

80377. Rohrs, H.W., G.J. Frost, G.B. Ellison, E.C. Richard and V. Vaida, "Fourier Transform Spectroscopy of Radicals," in *Advances in Molecular Structure Research* 1, 157-199 (1995), M. Hargittai and I. Hargittai, JAI Press, Inc., Greenwich CT. — FTIR FTUV/Visible Spectroscopy Simple Radicals Review

80378. Child, M.S., R.W. Field, D. Gauyacq and J.K.G. Watson, eds., "Molecular Rydberg Dynamics," *Phil. Trans. Roy. Soc. Lond. A* 355, 1475-1711 (1997). — Rydberg States Atoms, Molecules Dynamics Proceedings 15 Papers

80379. Held, A., and E.W. Schlag, "Zero Kinetic Energy Spectroscopy," *Acc. Chem. Res.* 31, 467-473 (1998). — ZEKE Spectroscopy Overview

80380. Walker, K.A., and M.C.L. Gerry, Laboratory Microwave Spectroscopy of Aluminum Cyanide," *Chem. Phys. Lett.* 301, 200-204 (1999). — AlCN FT Rotational Spectrum Constants AlNC Comparison

80381. Gerasimov, I., X. Yang and P.J. Dagdigian, "Laser Fluorescence Excitation Spectra of the AlNC and AlCN Isomers," *J. Chem. Phys.* 110, 220-228 (1999).

AlNC(A-X)
AlCN(A-X)
LIF Spectra
Assignments
Constants

(80832) Photoelectron Spectra, Constants, S/O Splitting, $D_0(As_2^-)$, EA(As_n)

As_n^-,n=1-5

(80833) Ion Photoelectron Spectrum, Constants, (a/X) Energy Splitting, EA(AsO), $D(AsO^-)$

AsO^-

80382. Hirota, E., "Plasma Diagnosis by High Resolution Spectroscopy of Transient Molecules," *Pure Appl. Chem.* 70, 1145-1150 (1998).

IR Diode Laser
Spectroscopy
High Resolution
CF_n ,SiH_n
Applications
Review

80383. von Busch, H., W. Demtroder, V. Dev, H.-A. Eckel, R. Grosskloss, M. Keil, H.-G. Kramer, T. Platz and H. Wenz, "High Resolution and High Sensitivity Laser Spectroscopy of Small Molecules and Clusters," *Phys. Scr.* 59, 147-151 (1999).

Highly Sensitive
Laser Spectroscopy
$CHCl_3$,CS_2 ,OCS
C_2H_2 ,C_2H_4 ,H_2S
Overtones, IVR
Methods
Review

80384. He, Y., M. Hippler and M. Quack, "High Resolution Cavity Ringdown Absorption Spectroscopy of Nitrous Oxide and Chloroform Using a Near-Infrared cw Diode Laser," *Chem. Phys. Lett.* 289, 527-534 (1998).

$CHCl_3(\nu_{CH})$
$N_2O(\nu_1+3\nu_3)$
Absorption
Cavity Ringdown
Absorption
Cross Sections

(80843) PFI/ZEKE Spectra, IPS

CH_4 ,CD_4

80385. Wu, C.Y.R., F.Z. Chen, D.L. Judge, X.-M. Hua and J. Caldwell, "Temperature-Dependent Absorption Strengths for Transitions from the Ground State to the Mutually Perturbed $A^1\Pi(v=1)$ and $d^3\Delta_1(v=5)$ States of CO," *J. Chem. Phys.* 110, 267-273 (1999).

CO(d-X),(5,0)
CO(A-X),(1,0)
Absorption
Cross Sections
Band Strengths
T Dependences

80386. Zhou, M., and L. Andrews, "Infrared Spectra of the CO_2^- and $C_2O_4^-$ Anions Isolated in Solid Argon," *J. Chem. Phys.* 110, 2414-2422 (1999).

CO_2^-,$(CO_2)_2^-$
FTIR Spectra
Frequencies
Matrix Study

80387. Lloyd, G.M., and P. Ewart, "High Resolution Spectroscopy and Spectral Simulation of C_2 Using Degenerate Four-Wave Mixing," *J. Chem. Phys.* 110, 385-392 (1999).

C_2(d-a)
High Resolution
DFWM Spectrum
Constants
C_2H_2/O_2 Flame

(80498) DFWM Spectrum, (0,0), (1,0) Bands, Rotational Line Analysis, Calculations — C_2(d-a)

(80487) Cavity Ringdown Absorption, Pulse Slit Nozzle Discharge, Sensitivities — C_2^-(B-X)
$C_6H(^2\Pi$-X)
$C_6H_2^+(^2\Pi$-X)

80388. Hirota, E., and Y. Endo, "High Resolution Spectroscopy of Transient Molecules and Its Applications to Molecular Dynamics," in *Vibration-Rotational Spectroscopy and Molecular Dynamics: Advances in Quantum Chemical and Spectroscopical Studies of Molecular Structures and Dynamics*, D. Papousek, ed., 9 Contributions, 562 pp., *Advanced Ser. Phys. Chem.* 9, 1-55 (1997).
FT Microwave Spectroscopy
Transient Species
C_2H,CHCN,C_2N
C_2O,C_2H_3,C_2H_5
C_3H_3,C_3H_5,FeCO
Review

80389. Yamaguchi, M., M. Furubayashi, S. Inomata and N. Washida, "Analysis of Laser Induced Fluorescence Spectra of the (B^2A''-X^2A'') Transition with Calculated Franck-Condon Factors of CH_2CFO," *Chem. Phys. Lett.* 298, 93-100 (1998).
CH_2CFO(B-X)
LIF Spectra
F.C. Factors
Assignments

80390. Pibel, C.D., A. McIlroy, C.A. Taatjes, S. Alfred, K. Patrick and J.B. Halpern, "The Vinyl Radical ($A^2A''\leftarrow X^2A'$) Spectrum Between 530 and 415 nm Measured by Cavity Ringdown Spectroscopy," *J. Chem. Phys.* 110, 1841-1843 (1999).
C_2H_3(A-X)
Absorption
Cavity Ringdown
Spectra
High Resolution

80391. De Lorenzi, A., S. Giorgianni and R. Bini, "High Resolution FTIR Spectroscopy of the C-Cl Stretching Mode of Vinyl Chloride," *Mol. Phys.* 96, 101-108 (1999).
$C_2H_3Cl(\nu_{CCl})$
FTIR Spectra
Constants

80392. Moazzen-Ahmadi, N., and R.T. Boere, "Infrared Laser Spectroscopy of CCO: The ν_1 Band of the $a^1\Delta$ Electronic State," *J. Chem. Phys.* 110, 955-959 (1999).
$C_2O(a),\nu_1$
IR Spectrum
Diode Laser
Band Origin

80393. Roth, D.A., M. Hepp, I. Pak and G. Winnewisser, "Unequivocal Laboratory Detection of CO Dimer Transitions in the Millimeter Wave Region," *Chem. Phys. Lett.* 298, 381-384 (1998).
$(CO)_2$
Millimeter Wave
Transitions

80394. Durig, J.R., Z. Yu, G.A. Guirgis, T.S. Little, M. Zhen and M.J. Lee, "Raman and Infrared Spectra, Conformational Stability, Normal Coordinate Analysis, Vibrational Assignment, and ab Initio Calculations of Difluoromethylcyclopropane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10460-10468 (1998).
c-$C_3H_5CHF_2$
IR,Raman
Spectra
Frequencies
Observed/
Calculated

(80848) Ion Photoelectron Spectra, A/X State Energy Splittings, EA(HO_2, *t*-$C_4H_9O_2$), D(*t*-C_4H_9OOH), Measurements — *t*-$C_4H_9OO^-$
HO_2^-

80395. Sinclair, W.E., D. Pfluger, H. Linnartz and J.P. Maier, "Rotationally Resolved ($A^2\Pi_g \leftarrow X^2\Pi_u$) Electronic Spectrum of Triacetylene Cation by Frequency Modulation Absorption Spectroscopy," *J. Chem. Phys.* 110, 296-303 (1999).

$C_6H_2^+$(A-X)
Absorption
Spectrum
D-Isotopes
Constants
Geometry

80396. Gerhards, M., M. Schiwek, C. Unterberg and K. Kleinermanns, "OH Stretching Vibrations in Aromatic Cations: Infrared/Photoinduced Rydberg Ionization Spectroscopy," *Chem. Phys. Lett.* 297, 515-522 (1998).

1,3-$C_6H_4(OH)_2^+$
Isomers
ν_{OH} Frequencies
Ground/Low-lying
States
Method

(80558) Ultraviolet Absorption Cross Sections

C_6H_5

80397. Fehrensen, B., M. Hippler and M. Quack, "Isotopomer-Selective Overtone Spectroscopy by Ionization Detected (IR+UV) Double Resonance of Jet Cooled Aniline," *Chem. Phys. Lett.* 298, 320-328 (1998).

$C_6H_5NH_2$
C_6H_5NHD
$2\nu_{NH}$ Overtone
Absorption
Assignments

80398. Devlin, F.J., and P.J. Stephens, "Ab Initio Density Functional Theory Study of the Structure and Vibrational Spectra of Cyclohexanone and Its Isotopomers," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 527-538 (1999).

c-$C_6H_{10}O_2$
d_0, d_4, d_6, d_{10}
Isotopomers
IR Spectra
Structural
Calculations
Frequencies

80399. Lee, S.K., and D.Y. Baek, "Vibronic Analysis of the Jet Cooled Emission Spectrum of *p*-Fluorobenzyl Radical in the ($D_1 \rightarrow D_0$) Transition," *Chem. Phys. Lett.* 301, 407-412 (1999).

$FC_6H_4CH_2(D_1\text{-}D_0)$
Emission Spectrum
Frequencies

80400. Engeln, R., G. von Helden, A.J.A. van Roij and G. Meijer, "Cavity Ringdown Spectroscopy on Solid C_{60}," *J. Chem. Phys.* 110, 2732-2733 (1999).

C_{60}(s)
IR Absorption
Cavity Ringdown
Spectrum

(80372) Solution Phosphorescent Spectra, Excited States

C_{60}, C_{70}

(80370) Spectroscopy, Structure, Energies, Review

$C_n, C_n^{\pm}$

80401. Friedrich, B., J.D. Weinstein, R. deCarvalho and J.M. Doyle, "Zeeman Spectroscopy of CaH Molecules in a Magnetic Trap," *J. Chem. Phys.* 110, 2376-2383 (1999).

CaH(B-X)
Zeeman/LIF
Spectra

80402. Gondal, M.A., M.A. Khan and M.H. Rais, "Observation of the ($a^3\Sigma_u^+$-$X^1\Sigma_g^+$) System of Calcium Dimer," *Nuovo Cimento D: Condensed Matter, At. Mol. Chem. Phys.* 20, 723-729 (1998).

Ca_2(a-X)
Emission Spectrum
Constants
T_0
$Ca(^3P_1)+Ca$
Formation

80403. Pushkarsky, M.B., T.A. Barckholtz and T.A. Miller, "The Fluorescence Depletion Spectroscopy of $CdCH_3$," *J. Chem. Phys.* 110, 2016-2028 (1999).

$CdCH_3$(A)
Fluorescence
Depletion Spectra
Vibronic Structure
Lifetimes

80404. Flaud, J.-M., T. Encrenaz and A. Omont, "Spectroscopy: Its Needs and Applications," *J. de Chim. Phys.* 95, 1771-1803 (1998).

$ClONO_2$,HNO_3
Spectroscopy
Applications
Atmospheric IR
Overview

80405. Bibinov, N.K., V.K. Davydov, A.A. Fateev, D.B. Kokh, E.V. Lugovoj, C. Ottinger and A.M. Pravilov, "The Transition Dipole Moment Function of the Chlorine ($E0_g^+(^3P_2)$-$B^3\Pi 0_u^+$) System," *J. Chem. Phys.* 109, 10864-10872 (1998).

Cl_2(E-B)
OODR Spectrum
Transition Moment
Curve

80406. Steimle, T.C., J.S. Robinson and D. Goodridge, "The Permanent Electric Dipole Moments of Chromium and Vanadium Mononitride: CrN and VN," *J. Chem. Phys.* 110, 881-889 (1999).

CrN(A-X)
VN(D-X)
Stark Spectra
Dipole Moments
First Row
MO,MN Comparisons

80407. Dachsel, H., R.J. Harrison and D.A. Dixon, "Multireference Configuration Interaction Calculations on Cr_2: Passing the One Billion Limit in MRCI/MRACPF Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 152-155 (1999).

Cr_2
Spectral Constants
Calculations
D_0

(80373) Infrared ν_{OD} Spectra, Assignments, Cavity Ringdown Method

$(D_2O)_n$,n=2-8

80408. Zhou, M., G.V. Chertihin and L. Andrews, "Reactions of Laser Ablated Iron Atoms with Carbon Monoxide: Infrared Spectra and Density Functional Calculations of Fe_nCO, $Fe(CO)_n$, and $Fe(CO)_n^-$ (n=1,2,3) in Solid Argon," *J. Chem. Phys.* 109, 10893-10904 (1998).

Fe_nCO,$Fe(CO)_n$
$Fe(CO)_n^-$,n=1-3
FTIR Spectra
Frequencies
Laser Ablated
Fe/CO
Matrix Study

80409. Korsgen, H., W. Urban and J.M. Brown, "The Infrared Spectrum of FeH_2, Studied in the Gas Phase by Laser Magnetic Resonance," *J. Chem. Phys.* 110, 3861-3869 (1999).

$FeH_2(X^5\Delta_g)$
LMR Spectrum
ν_3 Frequency
Constants
Geometry

80410. Harper, W.W., C.M. Klusek and D.J. Clouthier, "Spectroscopic Detection and Characterization of Iodogermylene, HGeI," *J. Chem. Phys.* 109, 9300-9305 (1998).

GeHI,GeDI
LIF Spectra
Structures
Fluorescence
Lifetimes

(80484) Intracavity Absorption, Densities, GeH_4 Discharge, Production Rates

GeH_2(A-X)

80411. Johnson, M.S., and B. Nelander, "High Resolution Gas Phase Spectroscopy with a Synchrotron Radiation Source," *Nuovo Cimento D: Condensed Matter, At. Mol. Chem. Phys.* 20, 449-462 (1998).

$HClO_4$,329 cm^{-1}
IBr,260 cm^{-1}
Mid- to Far IR
Spectroscopy
Synchrotron Source
High Resolution

80412. Flaud, J.-M., and A. Perrin, "High Resolution Infrared Spectroscopy and One-Dimensional Large Amplitude Motion in Asymmetric Tops: HNO_3 and H_2O_2," in *Vibration-Rotational Spectroscopy and Molecular Dynamics: Advances in Quantum Chemical and Spectroscopical Studies of Molecular Structures and Dynamics*, D. Papousek, ed., 9 Contributions, 562 pp., *Advanced Ser. Phys. Chem.* 9, 396-460 (1997).

HNO_3,H_2O_2
IR Spectroscopy
High Resolution
Large Amplitude
Motion Effects

(80866) Photoionization Efficiency Spectrum, IP(HOCl), $\Delta H_f(HOCl^+)$, PA(ClO), Measurements

HOCl

80413. Stimson, S., Y.-J. Chen, M. Evans, C.-L. Liao, C.Y. Ng, C.-W. Hsu and P. Heimann, "Rotational-Resolved Pulsed Field Ionization Photoelectron Bands for $H_2^+(X^2\Sigma_g^+, v^+=0,2,9$ and 11)," *Chem. Phys. Lett.* 289, 507-515 (1998).

H_2
PFI/PES
$H_2^+(v=0,2,9,11)$
Assignments
Rotational
Constants

80414. Fan, W.Y., N.T. Hunt, Z. Liu and P.B. Davies, "Infrared Laser Spectrum of High J Pure Rotational Transitions of $^4HeD^+$," *Chem. Phys. Lett.* 298, 222-226 (1998).

HeD^+
Rotational
Spectrum
Constants
v=0,1

80415. Shapiro, M., M.J.J. Vrakking and A. Stolow, "Nonadiabatic Wavepacket Dynamics: Experiment and Theory in IBr," *J. Chem. Phys.* 110, 2465-2473 (1999).

IBr(B/Y-X)
Wavepacket
Coupled States
Dynamics
fs Pump/Probe

80416. Hohm, U., "Analysis of the Vibrationally Resolved Polarizability Spectrum of I_2 in the Range of the ($B^3\Pi_u^+ \leftarrow X^1\Sigma_g^+$) Transition," *Mol. Phys.* 96, 7-13 (1999).

I_2(B-X)
Polarizability
Spectrum
($^1\Pi_u$,A-X)
Contributions
Analysis

80417. Xin, J., and L.M. Ziurys, "Structural Studies of Alkali Methylidyne Radicals: High Resolution Spectroscopy of NaCH and KCH($X^3\Sigma^-$)," *J. Chem. Phys.* 110, 3360-3367 (1999).

KCH(X)
NaCH(X)
Rotational
Spectra
Constants
D Isotopes

80418. Camacho, J.J., J.M.L. Poyato, A. Pardo and D. Reyman, "Analysis and Transition Probabilities of the ($A^1\Sigma^+ \rightarrow X^1\Sigma^+$) System of KH Excited by the 4880 A Line of the Argon Ion Laser," *J. Chem. Phys.* 109, 9372-9383 (1998).

KH(A-X)
LIF Spectrum
RKR P.E. Curves
F.C. Factors
A-Coefficients
$v'=7, J'=6$
Energy Transfer
Cross Sections

80419. Apponi, A.J., M.A. Brewster and L.M. Ziurys, "Rotational Spectroscopy of LiCCH($X^1\Sigma$) in Its Ground State and ν_5 Vibrational States," *Chem. Phys. Lett.* 298, 161-169 (1998).

$LiC_2H(X)$
$\nu_5=1$-3 States
Rotational
Spectral Constants
Structures

80420. Willson, S.P., and L. Andrews, "Characterization of the Reaction Products of Laser Ablated Late Lanthanide Metal Atoms with Dinitrogen: Matrix Infrared Spectra of LnN, $(LnN)_2$, and $Ln(NN)_x$ Molecules," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1311-1321 (1999).

$LnN,(LnN)_2$
FTIR Spectra
Ln=Tb,Dy,Ho,
Er,Tm,Yb,Lu
Frequencies
Matrix Study

80421. Ashfold, M.N.R., S.R. Langford, R.A. Morgan, A.J. Orr-Ewing, C.M. Western, C.R. Scheper and C.A. de Lange, "Resonance Enhanced Multiphoton Ionization and REMPI-Photoelectron Spectroscopy of Ammonia," *Eur. Phys. J. D* 4, 189-197 (1998).

NH_3
REMPI/PES
Rydberg State
Spectra

80422. Orphal, J., S. Dreher, S. Voigt, J.P. Burrows, R. Jost and A. Delon, "The Near-Infrared Bands of NO_2 Observed by High Resolution Fourier Transform Spectroscopy," *J. Chem. Phys.* 109, 10217-10221 (1998).

$NO_2(A-X)$
FTIR
9000-15000 cm^{-1}
Conical
Intersection
Region

(80563) Ultraviolet Absorption Cross Sections, Temperature Dependences

NO_2

(80871) Photoelectron Spectrum, NCN(b,a,X) Energy Spacings, NCN(b) Frequency

NCN^-

80423. Lee, C.-I., Y.-P. Lee, X. Wang and Q.-Z. Qin, "Isomers of N_2O_3: Observation of *trans-cis* N_2O_3 in Solid Ar," *J. Chem. Phys.* 109, 10446-10455 (1998).

N_2O_3
FTIR Spectra
Frequencies
Assignments
Isomers
Matrix Study

80424. Wang, J., H.-G. Kramer, M. Keil, H. von Busch and W. Demtroder, "Photodepletion Spectroscopy and Predissociation of the Na_3 $A'(^2A'_1)$ State," *Chem. Phys. Lett.* 301, 395-400 (1999).

$Na_3(A'-X)$
Photodepletion Spectrum
Vibronic Bands

80425. Barr, J.D., A. De Fanis, J.M. Dyke, S.D. Gamblin, N. Hooper, A. Morris, S. Stranges, J.B. West and T.G. Wright, "Study of the OH and OD Radicals with Photoelectron Spectroscopy Using Synchrotron Radiation," *J. Chem. Phys.* 110, 345-354 (1999).

OH,OD
PES Spectra
Rydberg State Assignments

80426. Carter, C.C., T.A. Miller, H.-S. Lee, P.P. Korambath, A.B. McCoy and E.F. Hayes, "High Resolution Electronic Spectroscopy of Kr.OH/D and an Empirical Potential Energy Surface," *J. Chem. Phys.* 110, 1508-1520 (1999).

OH.Kr(A-X)
OD.Kr(A-X)
LIF Spectra
Constants
P.E. Surfaces

80427. Bernath, P., M. Carleer, S. Fally, A. Jenouvrier, A.C. Vandaele, C. Hermans, M.-F. Merienne and R. Colin, "The Wulf Bands of Oxygen," *Chem. Phys. Lett.* 297, 293-299 (1998).

O_2
Wulf Bands
240-290 nm
$(A'^3\Delta_u-X^3\Sigma_g^-)$
Identification

80428. Evans, M., S. Stimson, C.Y. Ng, C.-W. Hsu and G.K. Jarvis, "Rotationally Resolved Pulsed Field Ionization Photoelectron Study of $O_2^+(B^2\Sigma_g^-, {}^2\Sigma_u^-; v^+=0\text{-}7)$ at 20.2-21.3 eV," *J. Chem. Phys.* 110, 315-327 (1999).

$O_2^+(B)$-$O_2(X)$
$O_2^+(^2\Sigma_u^-)$-$O_2(X)$
PFI-PES
$v'=0\text{-}7$
Ion Constants
Predissociation
Lifetimes
IP

80429. Ahmad, I.K., H. Ozeki and S. Saito, "Microwave Spectroscopic Detection of a Transient Phosphorus-Bearing Molecule, H_3PO," *J. Chem. Phys.* 110, 912-917 (1999).

PH_3O
Microwave Spectrum
Isotopomers
Rotational Constants
Geometry

80430. Gatehouse, B., T. Brupbacher and M.C.L. Gerry, "Fourier Transform Microwave Spectrum, Geometry, and Hyperfine Coupling Constants of Phosphenous Fluoride, OPF," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 560-567 (1999).

POF
Microwave Spectrum
Constants
Geometry

80431. Yamada, C., and E. Hirota, "The Microwave Spectrum of the Rubidium Monoxide RbO Radical," *J. Chem. Phys.* 110, 2853-2857 (1999).

$RbO(^2\Pi,X^2\Sigma)$
Rotational Spectra
Constants

(80874) Photoionization Efficiency Spectrum, IP

S_2O_2

80432. Kushto, G.P., M. Zhou, L. Andrews and C.W. Bauschlicher Jr, "An Infrared Spectroscopic and Density Functional Theoretical Investigation of the Reaction Products of Laser Ablated Scandium and Titanium Atoms with Nitric Oxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1115-1125 (1999).

ScNO,ScN,ScO
TiNO,TiN,TiO
FTIR Spectra
Ablated
Sc,Ti/NO
Matrix Study

80433. Zhou, M., and L. Andrews, "Reactions of Laser Ablated Vanadium Atoms with Nitric Oxide: Infrared Spectra and Density Functional Calculations on NVO, V-η^1-NO, V-(η^1-NO)$_2$, V-(η^1-NO)$_3$ and V-η^2-NO," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 478-484 (1999).

VNO,V(NO)$_n$
FTIR Spectra
Frequencies
Laser Ablation
V/NO
Matrix Study

80434. Lenzer, T., M.R. Furlanetto, K.R. Asmis and D.M. Neumark, "Zero Electron Kinetic Energy and Photoelectron Spectroscopy of the XeI^- Anion," *J. Chem. Phys.* 109, 10754-10766 (1998).

XeI,XeI^-
ZEKE,PES
Spectra
Low-lying States
Constants

27. EXCITED STATE LIFETIMES/QUENCHING

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

(80685) Reaction Dynamics, Channels to M + H_2(v,J) and MH + H, Conical Intersections, Erratum

M* + H_2

80435. Yuasa, K., S. Matayoshi and T. Sakurai, "Decay of Metastable Argon Atoms in the Afterglow Plasma," *Jpn. J. Appl. Phys.* 37, 6615-6619 (1998).

Ar*($1s_5$)
Decay Rates
Absorption
Measurements
Ar Plasma

80436. Rohrbacher, A., T. Ruchti, K.C. Janda, A.A. Buchachenko, M.I. Hernandez, T. Gonzalez-Lezana, P. Villarreal and G. Delgado-Barrio," A Combined Experimental-Theoretical Study of the Vibrational Predissociation and Product Rotational Distributions for High Vibrational Levels of $He^{79}Br_2$," *J. Chem. Phys.* 110, 256-266 (1999).

Br_2(B).He
v=10,39-48
Predissociation
Product
Br_2(B,v,J)
Distributions
Measurements

(80499) LIF Quenching Data, Flame Measurements

CCl*

(80738) P.E. Curves, Spectral Constants, Tunneling, Lifetimes

CH(B)

(80818) Rotational Energy Transfer, Fine Structure, Rate Constants

CN(A,v=3,N=60) + Ar

(80240) Dissociative Recombination Rate Constants, Branching Ratios, P.E. Curves

CN^+(a,X) + e^-

80437. Leu, G.-H., C.-L. Huang, S.-H. Lee, Y.-C. Lee and I.-C. Chen, "Vibrational Levels of the Transition State and Rate of Dissociation of Triplet Acetaldehyde," *J. Chem. Phys.* 109, 9340-9350 (1998).

$CD_3CDO(S_1)$
Fluorescence
Decays
S_1/T_1 Coupling
d_4, h_4 Dissociation
Thresholds

80438. Suzuki, T., and N. Hashimoto, "Predissociation of Acetylene from the A^1A_u State Studied by Absorption, Laser Induced Fluorescence, and H-Atom Action Spectroscopies," *J. Chem. Phys.* 110, 2042-2050 (1999).

$C_2H_2(A)$
Predissociation
Dynamics
Fluorescence
Quantum Yields
Electronic
Relaxation

80439. Zhong, Q., L. Poth and A.W. Castleman Jr, "Ultrafast Dissociation Dynamics of Acetone: A Revisit to the S_1 State and 3s Rydberg State," *J. Chem. Phys.* 110, 192-196 (1999).

$(CH_3)_2CO(S_1, 3s\text{-}X)$
CH_3CO
ps Dissociation
Lifetimes
D Isotopes
Dynamics

80440. Arrington, C.A., C. Ramos, A.D. Robinson and T.S. Zwier, "Ultraviolet Photochemistry of Diacetylene with Alkynes and Alkenes: Spectroscopic Characterization of the Products," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1294-1299 (1999).

$C_4H_2^* + C_2H_4, C_3H_6$
$C_4H_2^* + C_4H_2$
Reaction Products
C_6H_2, C_6H_4
C_7H_6, C_8H_2
R2PI Spectra

(80585) Lifetime, NO Fragment Yield, Supersonic Jet Measurements — $C_6H_5NO(S_2)$

(80402) Formation of $Ca_2(a)$, T_0, (a-X) Emission Spectrum, Constants — $Ca(^3P_1) + Ca$

(80403) Lifetimes, Fluorescence Depletion Spectra, Vibronic Structure — $CdCH_3(A)$

80441. Garcia-Vela, A., "On the Validity of the Time-Dependent Self-Consistent-Field Approach: Application to the Vibrational Predissociation of Cl_2-Ne," *Chem. Phys. Lett.* 290, 155-163 (1998).

$Cl_2(B,v).Ne$
Predissociation
Lifetimes
Product States
Calculations

80442. Cavero, V., J.-M. L'Hermite, G. Rahmat and R. Vetter, "$Cs(6D_{3/2}) + H_2 \rightarrow CsH + H$ Reaction. IV. Rotationally Resolved Total Cross Sections," *J. Chem. Phys.* 110, 3428-3436 (1999).

$Cs(6^2D_{3/2}) + H_2$
Reactive Quenching
Cross Sections
CsH(v,J)
Distributions
Measurements

(80410) Fluorescence Lifetimes, Spectra, Structures — GeHI,GeDI

(80247) Rydberg State Attachment, H^- Formation — $H_2^* + e^-$

(80249) Penning Ionization, Calculations, Erratum — $He(2^3S) + Ar$

(80250)	Penning/Associative Ionizations, Optical Trap, Low Temperature	$He^* + He^*$
80443.	Ogawa, T., and K. Ohno, "Classical Trajectory Calculations of Collision Energy Dependence of Total and Partial Penning Ionization Cross Sections for $He^*(2^3S) + N_2 \rightarrow He + N_2^+ + e^-$," *J. Chem. Phys.* 110, 3773-3780 (1999).	$He(2^3S) + N_2$ Penning Ionization Cross Sections Energy Dependences Calculations
80444.	Van Marter, T., and M.C. Heaven, "$I(^2P_{1/2}) + O_2$: Studies of Low Temperature Electronic Energy Transfer and Nuclear Spin-State Changing Collisions," *J. Chem. Phys.* 109, 9266-9271 (1998).	$I(^2P_{1/2}) + O_2$ $I(^2P_{1/2})$ F_2/F_3 Energy Transfer Rate Constants
(80800)	E-E Transfer, P.E. Surfaces, Crossings, Calculations	$I(^2P_{1/2}) + O_2$ $O_2(a) + I$
80445.	Hussain, A.N., and G. Roberts, "Wavepacket Dynamics of IBr Predissociation," *J. Chem. Phys.* 110, 2474-2488 (1999).	IBr(B) Predissociation Lifetimes B/Y Crossing Dynamics
80446.	Dietz, H., and V. Engel, "Single and Multiple Collision Effects Observed in the Femtosecond Spectroscopy of I_2-Rare Gas Collision Complexes: A Statistical Description," *J. Chem. Phys.* 110, 3335-3340 (1999).	I_2(B).Rg fs Pump/Probe Dissociating State Motion
80447.	Takayanagi, T., Y. Kurosaki, K. Sato, K. Misawa, Y. Kobayashi and S. Tsunashima, "Kinetic Studies on the $N(^2D,^2P) + CH_4$ and CD_4 Reactions: The Role of Nonadiabatic Transitions on Thermal Rate Constants," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 250-255 (1999).	$N(^2D) + CH_4, CD_4$ $N(^2P) + CH_4, CD_4$ Rate Constants Temperature Dependences
80448.	Umemoto, H., T. Asai, H. Hashimoto and T. Nakae, "Reactions of $N(2^2D)$ with H_2O and D_2O; Identification of the Two Exit Channels, NH(ND) + OH(OD) and H(D) + HNO(DNO)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 700-704 (1999).	$N(^2D) + H_2O, D_2O$ Channels NH(v,J),OH(v,J) H,D Product Energies
(80686)	Reaction Dynamics, Channels, Energies	$N(^2D) + H_2O$
80449.	Ritze, H.-H., W. Radloff and I.V. Hertel, "Decay of the Ammonia B-State Due to Nonadiabatic Coupling," *Chem. Phys. Lett.* 289, 46-52 (1998).	NH_3, ND_3(B,v) Lifetimes fs Pump/Probe B/A Coupling
80450.	Ottinger, C., and G. Shen, "A Beam Experiment on the Energy Transfer Reaction $NO(a^4\Pi) + NO(X^2\Pi) \rightarrow NO(X^2\Pi) + NO(A^2\Sigma^+)$," *Chem. Phys. Lett.* 289, 231-240 (1998).	NO(a) + NO Cross Section NO(A) Product Beam Experiment
(80251)	Charge Transfer, N_2^+(B) Product, (B-X) Emission	$N_2(A) + N^+$

80451. De Benedictis, S., G. Dilecce and M. Simek, "Excitation and Decay of $N_2(B^3\Pi_g,v)$ States in a Pulsed Discharge: Kinetics of Electrons and Long-Lived Species," *J. Chem. Phys.* 110, 2947-2962 (1999).

$N_2(B,v)+N_2$
Quenching
Rate Constants
N_2 Discharge
Kinetic Modeling

(80253) Associative Ionization, Polarization Anisotropy Effects

Na^*+Na^*

(80254) Penning Ionization, Well Depth, $N_2^+(v)$ Product Distribution, $N_2^+(A)$ Intermediate

$Ne(^3P_{0,2})+N_2$

(80569) Rate Constants, $D(NiSO_2)$, Measurements

$Ni(a^3D_J)+SO_2+Ar$

80452. Tsurumaki, H., Y. Fujimura and O. Kajimoto, "Stereodynamics of the Reactions of (^1D) with C_2H_4 and C_2H_6," *Chem. Phys. Lett.* 301, 145-152 (1999).

$O(^1D)+C_2H_4$
$O(^1D)+C_2H_6$
Cross Sections
Stereodynamics

(80609) Crossed Beams, Product D Velocity Mapping

$O(^1D)+D_2$

(80752) P.E. Surface, Interpolation Method

$O(^1D)+H_2$

(80694) Reaction Dynamics, Cross Sections, NO(v) Product Distributions

$O(^1D)+N_2O$

80453. Parlant, G., and D.R. Yarkony, "A Theoretical Analysis of the State-Specific Decomposition of $OH(A^2\Sigma^+,v',N',F_1/F_2)$ Levels, Including the Effects of Spin-Orbit and Coriolis Interactions," *J. Chem. Phys.* 110, 363-376 (1999).

OH(A,v,N)
Predissociation
Rates
Product $O(^3P_J)$
Branching Ratios
Calculations

80454. Hwang, E.S., A. Bergman, R.A. Copeland and T.G. Slanger, "Temperature Dependence of the Collisional Removal of $O_2(b^1\Sigma_g^+,v=1$ and 2) at 110-260 K, and Atmospheric Applications," *J. Chem. Phys.* 110, 18-24 (1999).

$O_2(b)_{v=1,2}+M$
Quenching
Rate Constants
T Dependence
$M=CO_2,N_2,O_2$

(80428) Predissociation Lifetimes, $O_2^+(B)$-$O_2(X)$, $O_2^+(^2\Sigma_u^-)$-$O_2(X)$ PFI-PES Spectra, $v'=0$-7, Ion Constants, IP

$O_2^+(B,^2\Sigma_u^-)$

80455. Liu, C., S. Zou, J. Guo, Y. Gu, D. Cao and Y. Chu, "Quenching Rate Constants for Metastable Molecule $PCl(b^1\Sigma^+,v=0)$," *Chinese Sci. Bull.* 42, 1433-1435 (1997).

PCl(b)+M
Quenching
Rate Constants
M=24 Molecules

80456. Xuan, C.N., and A. Margani, "Collision Induced Deactivation of $PH_2(A^2A_1;v'_2=1,0)$ and $PH_2(X^2B_1;v''_2=1)$ by Diatomic Molecules," *J. Chem. Phys.* 109, 9417-9429 (1998).

$PH_2(A,v=1,0)+M$
$PH_2(X,v=1)+M$
Relaxation
Rate Constants
$M=CO,H_2,NO,N_2$

(80616) RbH(T,v,J) Product Energy Distributions, Measurements

$Rb(5^2D,7^2S)+H_2$

80457. Lee, S.-H., and K. Liu, "Isotope Effects and Excitation Functions for the Reactions of $S(^1D)+H_2$, D_2 and HD," *Chem. Phys. Lett.* 290, 323-328 (1998).

$S(^1D)+H_2,HD,D_2$
Rate Constants
Collisional Energy Effects
Insertion
Isotope Effects

(80702) Reaction Dynamics, Spin Effects, Channels

$Sc^+(^1D)+H_2O$
$V^+(^3F)+H_2O$

(80755) Lifetimes, P.E. Curves, Transition Probabilities, Spectral Constants, Calculations

$SiC^-(B^2\Sigma^+,v)$

80458. Hirano, I., J. Yoda, F.-L. Hong, K. Okumura and A. Onae, "Determination of Collisional Quenching Rate for the $4D_{3/2}$ State in Sr^+," *Jpn. J. Appl. Phys.* 37, 5767-5771 (1998).

$Sr^+(4^2D_{3/2})+He$
Quenching Rate
Ion Trap

(80703) Reaction Dynamics, ZnH, ZnD(v,J) Product Distributions, Data/Theory Comparisons

$Zn^*(^3P)+H_2,HD,D_2$

28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

(80389) F.C. Factors, LIF Spectrum, Assignments

$CH_2CFO(B-X)$

(80405) Transition Moment Curve, OODR Spectrum

$Cl_2(E-B)$

80459. Donnelly, D., A. Hibbert and K.L. Bell, "Oscillator Strengths for Transitions in Singly Ionized Copper," *Phys. Scr.* 59, 32-48 (1999).

Cu^+
Transition Probabilities
Calculations

80460. He, G., and R.G. Macdonald, "Experimental Determination of the ν_1 Fundamental Vibrational Transition Moment for HNC," *Chem. Phys. Lett.* 301, 175-182 (1999).

HNC,ν_1
Transition Moment

(80418) F.C. Factors, A-Coefficients, LIF Spectrum, Measurements

KH(A-X)

80461. Palmeri, P., and J.-F. Wyart, "Fine Structure and Transition Probabilities in Neutral Molybdenum," *Phys. Scr.* 58, 445-456 (1998).

Mo
Transition Probabilities
Calculations

(80811) Einstein A-Factors, Infrared Transitions

NO(v)

80462. Nagarajan, K., and N. Rajamanickam, "Franck-Condon Factors and *r*-Centroids of Certain Band Systems of Astrophysical Molecules SO and TiO," *Astrophys. Space Sci.* 259, 421-425 (1998).

SO(b-X)
TiO(f-a;e-d)
F.C. Factors
r-Centroids
Calculations

(80755) Transition Probabilities, P.E. Curves, Spectral Constants, Calculations — SiC^-(B-A,B-X)

29. LINESHAPES/STRENGTHS

80463. Herman, R.M., ed., *"Spectral Lineshapes: Volume 10,"* Proceedings of the 14th International Conference Held at State College PA, June 1998, 102 Papers, *Am. Inst. Phys. Conf. Proc.* 467, 566 pp. (1999).
Spectral Lineshapes
Atoms,Molecules
Plasma
Conference
Proceedings

(80385) Band Strengths, Absorption Cross Sections, Temperature Dependences
CO(d-X),(5,0)
CO(A-X),(1,0)

80464. Temsamani, M.A., J.-M. Champion and S. Oss, "Infrared Transition Intensities in Acetylene: An Algebraic Approach," *J. Chem. Phys.* 110, 2893-2902 (1999).
C_2H_2
Absolute
IR Intensities
$\leq$10,000 cm^{-1}
Model

80465. Musielok, J., "Regularities of Line Strengths in Spectra of N, F and Ne^+," *Acta Phys. Pol. A* 94, 13-23 (1998).
F,N(3s-3p)
Ne^+(3p-3d)
Line Strengths
Experiment/Theory
Comparisons

(80728) Infrared Intensities, Vibrational Energy Levels, Calculations
HOCl

80466. Lucchesini, A., M. De Rosa, C. Gabbanini and S. Gozzini, "Diode Laser Spectroscopy of Oxygen Electronic Band at 760 nm," *Nuovo Cimento D: Condensed Matter, At. Mol. Chem. Phys.* 20, 253-260 (1998).
O_2(b-X),(0,0)
Broadening
Coefficients
Wavelength
Modulation
Measurements

80467. Pope, R.S., P.J. Wolf, G.P. Perram and J.J. Cornicelli, "Collision Broadening of Spectral Lines in the ($X^3\Sigma_g^- \rightarrow b^1\Sigma_g^+$) System of O_2," in *Fourier Transform Spectroscopy: Eleventh International Conference*, J.A. de Haseth, ed., 152 Papers, 753 pp., Presented in Athens GA, August 1997, *Am. Inst. Phys. Conf. Proc.* 430, 715-718 (1998).
O_2(b-X),(0,0)
Broadening
Coefficients
Rg,CO,CO_2
O_2,SF_6

30. ANALYSIS/MONITORING TECHNIQUES

(See also Section 20 for Atmospheric Measurement Methods and Section 32 for Mapping and Tomographic Methods)

80468. Huang, M., T. Shirasaki, A. Hirabayashi and H. Koizumi, "Microliter Sample Introduction Technique for Microwave-Induced Plasma Mass Spectrometry," *Anal. Chem.* 71, 427-432 (1999).
Microwave Plasma
Mass Analysis
Microliter Samples
Monitoring
Method

(80510)	C_3-C_{12} Hydrocarbons, Flame Profiles, CH_4/Air Jet, Monitoring	Microprobe/ Photoionization Mass Analysis
80469.	Butcher, D.J., D.E. Goeringer and G.B. Hurst, "Real-Time Determination of Aromatics in Automobile Exhaust by Single-Photon Ionization Ion Trap Mass Spectrometry," *Anal. Chem.* 71, 489-496 (1999).	Photoionization/ Mass Analysis Aromatics Automobile Exhaust Monitor
80470.	Leach, J.J., L.A. Allen, D.B. Aeschliman and R.S. Houk, "Calibration of Laser Ablation Inductively Coupled Plasma Mass Spectrometry Using Standard Additions with Dried Solution Aerosols," *Anal. Chem.* 71, 440-445 (1999).	Laser Ablated ICP/MS Calibration Method
80471.	Peng, W.X., K.W.D. Ledingham, R.P. Singhal and T. McCanny, "Urban Air Pollution Monitoring: Laser Based Procedure for the Detection of Carbon Monoxide Gas," *Analyst* 123, 1035-1039 (1998).	REMPI CO (2+1) Mode Monitor Sensitivity
80472.	Heger, H.J., R. Zimmermann, R. Dorfner, M. Beckmann, H. Griebel, A. Kettrup and U. Boesl, "On-Line Emission Analysis of Polycyclic Aromatic Hydrocarbons down to pptv Concentration Levels in the Flue Gas of an Incineration Pilot Plant with a Mobile Resonance-Enhanced Multiphoton Ionization Time-of-Flight Mass Spectrometer," *Anal. Chem.* 71, 46-57 (1999).	REMPI/TOFMS $C_{10}H_8$,PAHS Incinerator On-line Flue Gas Monitor
(80717)	Combustion Applications, Techniques, Review	Laser Diagnostics
(80278)	CH, OH Spectral Emission Method, CH_4/Air and C_2H_2/O_2 Flames	Equivalence Ratio Monitor
(80328)	Gas Turbine Exhaust, Temperatures, Monitoring	FTIR Emission CO,CO_2
(80351)	Soot Volume Fractions, Cavity Ringdown Calibration	LII Monitor
80473.	Barat, R.B., and A.T. Poulos, "Detection of Mercury Compounds in the Gas Phase by Laser Photo-Fragmentation/Emission Spectroscopy," *Appl. Spectrosc.* 52, 1360-1363 (1998).	Laser Photolysis/ Emission $HgCl_2$,HgI_2 $Hg(CH_3)Cl$ Monitoring Method
80474.	Woskov, P.P., K. Hadidi, M.C. Borras, P. Thomas, K. Green and G.J. Flores, "Spectroscopic Diagnostics of an Atmospheric Microwave Plasma for Monitoring Metals Pollution," *Rev. Sci. Instrum.* 70, 489-492 (1999).	Emission Microwave Discharge Atom Monitor N_2^+(B-X),(0,0),T_{rot} Fe*,T_{exc} Plasma Characterization

80475.	Castle, B.C., K. Talabardon, B.W. Smith and J.D. Winefordner, "Variables Influencing the Precision of Laser Induced Breakdown Spectroscopy Measurements," *Appl. Spectrosc.* 52, 649-657 (1998).	Laser Induced Breakdown Spectra Cu Spectral Emission Precision Variables
80476.	Dudragne, L., Ph. Adam and J. Amouroux, "Time-Resolved Laser Induced Breakdown Spectroscopy: Application for Qualitative and Quantitative Detection of Fluorine, Chlorine, Sulfur and Carbon in Air," *Appl. Spectrosc.* 52, 1321-1327 (1998).	Laser Induced Breakdown Spectra F,Cl,S,C Atomic Emission Analysis
80477.	Bovensmann, H., J.P. Burrows, M. Buchwitz, J. Frerick, S. Noel, V.V. Rozanov, K.V. Chance and A.P.H. Goede, "Scanning Imaging Absorption Spectrometer for Atmospheric Chartography: Mission Objectives and Measurement Modes," *J. Atmos. Sci.* 56, 127-150 (1999).	Atmospheric Absorption Monitor Species Profiles New Spectrometer 240-2380 nm
(80504)	Flame Profile Monitoring, CH_4/Air, Heat Release Rates	Absorption HCO
80478.	Brandenburger, U., T. Brauers, H.-P. Dorn, M. Hausmann and D.H. Ehhalt, "In Situ Measurements of Tropospheric Hydroxyl Radicals by Folded Long-Path Laser Absorption During the Field Campaign POPCORN," *J. Atm. Chem.* 31, 181-204 (1998).	DOAS CH_2O,$C_{10}H_8$ OH,SO_2 Atmospheric Measurements
(80597)	Monitoring Method, $SiCl_4 + h\nu$, High Temperatures, Kinetic Model	Absorption Cl,Si
80479.	Hofzumahaus, A., U. Aschmutat, U. Brandenburger, T. Brauers, H.-P. Dorn, M. Hausmann, M. Hessling, F. Holland, C. Plass-Dulmer and D.H. Ehhalt, "*J. Atm. Chem.* 31, 227-246 (1998).	DOAS,LIF OH Atmospheric Monitoring Comparisons
80480.	Allen, M.G., "Diode Laser Absorption Sensors for Gas-Dynamic and Combustion Flows," *Measurement Sci. Technol.* 9, 545-562 (1998).	Absorption Diode Lasers Combustion Monitor
80481.	Mihalcea, R.M., D.S. Baer and R.K. Hanson, "A Diode Laser Absorption Sensor System for Combustion Emission Measurements," *Measurement Sci. Technol.* 9, 327-338 (1998).	Absorption Diode Laser CO,CO_2,O_2 NO,N_2O,H_2O Combustion Emissions Monitor

80482.	Mihalcea, R.M., D.S. Baer and R.K. Hanson, "Advanced Diode Laser Absorption Sensor for In Situ Combustion Measurements of CO_2, H_2O and Gas Temperature," *Int. Symp. Combust.* 27, 95-101 (1998).	Absorption Diode Laser T,CO_2,H_2O C_2H_4/Air Flame Monitoring
80483.	Furlong, E.R., D.S. Baer and R.K. Hanson, "Real-Time Adaptive Combustion Control Using Diode Laser Absorption Sensors," *Int. Symp. Combust.* 27, 103-111 (1998).	Absorption Diode Laser T,H_2O Dump Combustor Adaptive Feedback Controller
80484.	Kawasaki, H., J. Kida, K. Sakamoto, T. Fukuzawa, M. Shiratani and Y. Watanabe, "Similarities in Spatial Distributions of Absolute GeH_2 Density, Radical Production Rate and Particle Amount in GeH_4 Radiofrequency Discharges," *Jpn. J. Appl. Phys. Lett. B* 37, L475-L477 (1998).	Absorption GeH_2(A-X) Intracavity GeH_4 Discharge Densities Production Rates
(80296)	Diesel Engine, Exhaust Gas Measurements	Absorption SO_2
80485.	Engeln, R., G. Berden, R. Peeters and G. Meijer, "Cavity Enhanced Absorption and Cavity Enhanced Magnetic Rotation Spectroscopy," *Rev. Sci. Instrum.* 69, 3763-3769 (1998).	Absorption Cavity Enhanced Method O_2(b-X),(2,0-0) Optical Rotation
80486.	Crosson, E.R., P. Haar, G.A. Marcus, H.A. Schwettman, B.A. Paldus, T.G. Spence and R.N. Zare, "Pulse-Stacked Cavity Ringdown Spectroscopy," *Rev. Sci. Instrum.* 70, 4-10 (1999).	Absorption Cavity Ringdown Pulse Stacking Technique Enhanced Sensitivities
(80384)	Cavity Ringdown, Cross Sections	Absorption $CHCl_3(\nu_{CH})$ $N_2O(\nu_1+3\nu_3)$
(80503)	Flame Profiles, CH_4/Air, Monitoring	Intracavity Absorption/ Ringdown Methods $^1CH_2$,HCO,OH
80487.	Motylewski, T., and H. Linnartz, "Cavity Ringdown Spectroscopy on Radicals in a Supersonic Slit Nozzle Discharge," *Rev. Sci. Instrum.* 70, 1305-1312 (1999).	Absorption Cavity Ringdown C_2^-(B-X) $C_6H(^2\Pi$-X) $C_6H_2^+(^2\Pi$-X) Pulse Slit Nozzle Discharge Sensitivities

80488. Levenson, M.D., B.A. Paldus, T.G. Spence, C.C. Harb, J.S. Harris Jr and R.N. Zare, "Optical Heterodyne Detection in Cavity Ringdown Spectroscopy," *Chem. Phys. Lett.* 290, 335-340 (1998).

Absorption
Cavity Ringdown
H_2O
Heterodyne
Detection

80489. Schulz, K.J., and W.R. Simpson, "Frequency Matched Cavity Ringdown Spectroscopy," *Chem. Phys. Lett.* 297, 523-529 (1998).

Absorption
cw Cavity
Ringdown Spectrum
H_2O,NO_3

80490. Hemmerling, B., W. Hubschmid and A. Stampanoni-Panariello, "Temperature and Mixture Fraction Measurements in Gases by Laser Induced Electrostrictive Gratings," *Int. Symp. Combust.* 27, 69-75 (1998).

IR Laser Induced
Grating
Absorption
T,Densities
Monitoring Method

80491. Frejafon, E., J. Kasparian, P. Rambaldi, B. Vezin, V. Boutou, J. Yu, M. Ulbricht, D. Weidauer, B. Ottobrini, E. de Saeger, B. Kramer, T. Leisner, P. Rairoux, L. Woste and J.P. Wolf, "Laser Applications for Atmospheric Pollution Monitoring," *Eur. Phys. J. D* 4, 231-238 (1998).

3-D Atmospheric
LIDAR Monitor
Gases/
Aerosols

(80277) Doped Fuel LIF Method, Raman Calibration Method

Fuel/Air
Monitor

(80324) Flue Gas Alkali Emissions, Absorption Control Monitor

Photofragment
LIF,Alkalis

(80499) Species Profiles Monitoring, CH_4/CH_3Cl/Air and CH_4/CH_2Cl_2/Air Flames, CCl* Quenching Data

LIF,CCl,CH,NO

80492. Suzuki, C., K. Sasaki and K. Kadota, "Surface Kinetics of CF_x Radicals and Fluorine Atoms in the Afterglow of High-Density C_4F_8 Plasmas," *Jpn. J. Appl. Phys.* 37, 5763-5766 (1998).

CF,CF_2 LIF
F VUV Absorption
Measurements
C_4F_8 Discharge

(80500) Flame Profiles Monitoring, CH_4/O_2/NO, Kinetic Model Comparisons

LIF/Absorption
CH,CH_3,CN,NO

(80502) Monitoring, $CH_4/O_2/N_2$ Flames

LIF,HCO

80493. Daugey, N., J. Shu, I. Bar and S. Rosenwaks, "Nitrobenzene Detection by One-Color Laser Photolysis/Laser Induced Fluorescence of NO (v''=0-3)," *Appl. Spectrosc.* 53, 57-64 (1999).

$C_6H_5NO_2$
Monitor
Laser Photolysis
LIF,NO
Detection Method
Sensitivity

80494. Versluis, M., G. Juhlin, O. Andersson and M. Alden, "Two Dimensional Two-Phase Water Detection Using a Tunable Excimer Laser," *Appl. Spectrosc.* 52, 343-347 (1998).

2-Photon LIF
SRS
2-D Gas/Liquid
H_2O Phases
Monitor

80495. Fong, C., and W.H. Brune, "A Laser Induced Fluorescence Instrument for Measuring Tropospheric NO_2," *Rev. Sci. Instrum.* 68, 4253-4262 (1997).

LIF
NO_2
Direct Method
Atmospheric
Monitor

80496. Holland, F., U. Aschmutat, M. Hessling, A. Hofzumahaus and D.H. Ehhalt, "Highly Time Resolved Measurements of OH During POPCORN Using Laser Induced Fluorescence Spectroscopy," *J. Atm. Chem.* 31, 205-225 (1998).

LIF
OH(A-X)
Atmospheric
Measurements
High Resolution
High Specificity

(80511) C_3H_6/O_2/Ar Species Profiles, Molecular Beam Sampling/Mass Analysis of Hydrocarbons

LIF,OH
Raman,CO,H_2

80497. Funk, J.-M., T. Michelis, R. Eck and A. Materny, "Nanosecond Time-Resolved Resonance CARS Spectroscopy Using the Scanning Multichannel Technique," *Appl. Spectrosc.* 52, 1541-1553 (1998).

ns CARS
PAHS
Organics
Monitor

80498. Ryu, J.-s., and J.W. Hahn, "Calculations of the Rotational Lines and Their Strength for the Swan Band of C_2 Molecules: A Study on the Degenerate Four Wave Mixing Spectrum," *Jpn. J. Appl. Phys.* 37, 6217-6222 (1998).

DFWM
C_2(d-a)
(0,0),(1,0) Bands
Rotational
Line Spectrum
Calculations

31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

80499. Devynck, P., P. Desgroux, L. Gasnot, E. Therssen and J.F. Pauwels, "CCl, CH and NO LIF Measurements in Methane/Air Flames Seeded with Chlorinated Species: Influence of CH_3Cl and CH_2Cl_2 on CCl and NO Formation," *Int. Symp. Combust.* 27, 461-468 (1998).

CCl,CH,NO
Species Profiles
CH_4/CH_3Cl/Air
CH_4/CH_2Cl_2/Air
LIF Monitor
CCl*
Quenching Data

80500. Juchmann, W., H. Latzel, D.I. Shin, G. Peiter, T. Dreier, H.-R. Volpp, J. Wolfrum, R.P. Lindstedt and K.M. Leung, "Absolute Radical Concentration Measurements and Modeling of Low Pressure CH_4/O_2/NO Flames," *Int. Symp. Combust.* 27, 469-476 (1998).

CH,CH_3,CN,NO
Flame Profiles
CH_4/O_2/NO
LIF/Absorption
Monitoring
Kinetic Model
Comparisons

80501. Walsh, K.T., M.B. Long, M.A. Tanoff and M.D. Smooke, "Experimental and Computational Study of CH, CH* and OH* in an Axisymmetric Laminar Diffusion Flame," *Int. Symp. Combust.* 27, 615-623 (1998).

CH,CH*,OH*
Species Profiles
Laminar
Diffusion Flame
CH_4/Air
Measurements
Model Comparisons

80502. Diau, E.W.-G., G.P. Smith, J.B. Jeffries and D.R. Crosley, "HCO Concentration in Flames via Quantitative Laser Induced Fluorescence," *Int. Symp. Combust.* 27, 453-460 (1998).

HCO
Species Profiles
$CH_4/O_2/N_2$
Flames
LIF Monitor

80503. Lozovsky, V.A., I. Derzy and S. Cheskis, "Radical Concentration Profiles in a Low Pressure Methane/Air Flame Measured by Intracavity Laser Absorption and Cavity Ringdown Spectroscopy," *Int. Symp. Combust.* 27, 445-452 (1998).

$^1CH_2$,HCO,OH
Species Profiles
CH_4/Air Flame
Intracavity
Absorption/
Cavity Ringdown
Methods

80504. Tolocka, M.P., and J.H. Miller, "Measurements of Formaldehyde Concentrations and Formation Rates in a Methane/Air, Nonpremixed Flame and Their Implications for Heat Release Rate," *Int. Symp. Combust.* 27, 633-640 (1998).

HCHO
Absorption
Flame Profiles
CH_4/Air
Heat Release
Rates

80505. Roesler, J.F., "An Experimental and Two-Dimensional Modeling Investigation of Combustion Chemistry in a Laminar Non-Plug Flow Reactor," *Int. Symp. Combust.* 27, 287-293 (1998).

CH_4/O_2
$CO/O_2/H_2O$
Laminar Flow
Reactor Profiles
Non Plug Flow
Conditions

(80201) Turbulent, Rayleigh/Raman/LIF, Temperatures, Measurements

CH_4/Air
Species Profiles

80506. Werner, J.H., and T.A. Cool, "The Combustion of Trichloroethylene Studied with Vacuum Ultraviolet Photoionization Mass Spectrometry," *Int. Symp. Combust.* 27, 413-423 (1998).

Species Profiles
$CH_4/C_2HCl_3/O_2$
Flame Sampling
VUV Mass Analyzer
Products
Kinetics

80507. Li, S.C., and F.A. Williams, "Formation of NO_x, CH_4 and C_2 Species in Laminar Methanol Flames," *Int. Symp. Combust.* 27, 485-493 (1998).

CH_4,C_2H_2,C_2H_4
C_2H_6,NO_x
Species Profiles
CH_3OH/Air
Measurements
Modeling

(80482)	C_2H_4/Air Flame, Diode Laser Absorption Monitoring	CO_2, H_2O Temperatures
80508.	McEnally, C.S., and L.D. Pfefferle, "Comparison of Non-Fuel Hydrocarbon Concentrations Measured in Coflowing Nonpremixed Flames Fueled with Small Hydrocarbons," *Combust. Flame* 117, 362-372 (1999).	Hydrocarbon Flames Probe Sampling Mass Analysis C_2-C_{12} Product Hydrocarbons
80509.	Werner, J.H., and T.A. Cool, "Flame Sampling Photoionization Mass Spectrometry of Dichloroethenol," *Chem. Phys. Lett.* 290, 81-87 (1998).	$C_2H_2Cl_2$ CCl_2CHOH Flame Sampling Mass Analyzer $CH_4/O_2/C_2HCl_3$ IP(CCl_2CHOH)
80510.	McEnally, C.S., L.D. Pfefferle, R.K. Mohammed, M.D. Smooke and M.B. Colket, "Mapping of Trace Hydrocarbon Concentrations in Two-Dimensional Flames Using Single-Photon Photoionization Mass Spectrometry," *Anal. Chem.* 71, 364-372 (1999).	C_3-C_{12} Hydrocarbons Flame Profiles Microprobe/ Photoionization Mass Analysis Monitor CH_4/Air Jet
80511.	Atakan, B., A.T. Hartlieb, J. Brand and K. Kohse-Hoinghaus, "An Experimental Investigation of Premixed Fuel-Rich Low Pressure Propene/Oxygen/Argon Flames by Laser Spectroscopy and Molecular-Beam Mass Spectrometry," *Int. Symp. Combust.* 27, 435-444 (1998).	$C_3H_6/O_2/Ar$ Species Profiles LIF/Molecular Beam Sampling Mass Analysis
(80557)	Species Profiles, Molecular Beam Mass Analysis, Kinetics	$H_2/C_4H_9OCH_3/O_2$
(80483)	Diode Laser Absorption Monitoring, Dump Combustor, Adaptive Feedback Controller	H_2O Temperatures
80512.	Werner, J.H., and T.A. Cool, "Kinetic Model for the Decomposition of Dimethyl Methyl Phosphonate in a Hydrogen/Oxygen Flame," *Combust. Flame* 117, 78-98 (1999).	Phosphorus Flame Chemistry $H_2/O_2/(CH_3)_3PO_3$ Species Profiles Kinetic Modeling
(80257)	Sn Flame Chemistry, Probe Sampling/Mass Analysis, $SnOH^+ + e^-$ Rate Constant, ΔH_f, D_0 ($SnOH^+$)	Sn,Sn^+,SnO $SnOH^+$ Profiles

32. MAPPING/TOMOGRAPHIC METHODS

(80170)	Mapping, Counterflow H_2, N_2/Air Diffusion Flames, Strained by an Impinging Microjet, Extinction, Re-ignition	2-D Temperatures
(80197)	Rayleigh Scattering, Turbulent 3-D Flame Structure, Preheat Zone Thickness	2-D 2-Plane Temperatures

(80199)	Turbulent CH_4/Air, Planar Rayleigh Scattering, Measurements	3-D Temperature Gradients
(80198)	Simultaneous Rayleigh/LIF Measurements, Turbulent CH_4/Air, Highly Stretched	2-D Temperatures LIF,CH
(80129)	Shock Tunnel Measurements	Temperatures PLIF,NO
(80202)	Turbulent CH_4/Air Flame Structure, Swirl Stabilized, Quenching	2-D Temperatures 2-D LIF,OH
(80230)	Lifted Jet Diffusion Flame Flowfield, PIV, Leading Edge, CH_4/Air	PLIF,CH,OH
(80604)	2-D Imaging, Product Energies, $CH_3I + h\nu$, Dynamics, D(CH_3I)	CH_3(T,v,J) $I(^2P_{1/2,3/2})$
(80613)	2-D Imaging, Product Vector Correlations, $NO_2 + h\nu$, Data/Theory Comparisons	NO(X,v,J)
80513.	Paul, P.H., and H.N. Najm, "Planar Laser Induced Fluorescence Imaging of Flame Heat Release Rate," *Int. Symp. Combust.* 27, 43-50 (1998).	Imaging Heat Release PLIF,OH,CH_2O Method
(80227)	Flow Visualization, Flame/Vortex Interactions, Counterflow Burner, Images	PLIF,OH
(80224)	Flow Visualization Images, CH_4/Air, Swirl Effects	PLIF,OH
(80169)	Counterflow CH_4,N_2/Air Diffusion Flames, Oscillations, Extinction, Stretch Effects	2-D PLIF,OH
(80208)	C_3H_8 /Air Turbulent Velocities, Measurements	PIV,PLIF OH
(80193)	H_2/Air, Flame/Vortex Interactions, Extinctions	PLIF,OH
80514.	Bingham, D.C., F.C. Gouldin and D.A. Knaus, "Crossed-Plane Laser Tomography: Direct Measurement of the Flamelet Surface Normal," *Int. Symp. Combust.* 27, 77-84 (1998).	Laser Tomography Turbulent Flames Boundaries Monitoring Method
80515.	McMackin, L., R.J. Hugo, K.P. Bishop, E.Y. Chen, R.E. Pierson and C.R. Truman, "High Speed Optical Tomography System for Quantitative Measurement and Visualization of Dynamic Features in a Round Jet," *Experiments Fluids* 26, 249-256 (1999).	Tomography Optical Heated Jet Visualization
(80206)	Turbulent CH_4, C_3H_8, H_2/Air, Displacement Speeds, Strain Rates	PIV/Laser Tomography
(80163)	OH Flame Structure, H_2/Liquid O_2 Stabilization	Tomographic Measurements

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

80516.	Scudieri, F., and M. Bertolotti, eds., *"Photoacoustic and Photothermal Phenomena,"* Proceedings of the 10th International Conference, Held in Rome, Italy, August 1998, 212 Papers, *Am. Inst. Phys. Conf. Proc.* 463, 691 pp. (1999).	Optoacoustic Optothermal Techniques Conference Proceedings

34. FLAME KINETIC MODELING

(See also Section 10 for Kinetic Modeling of Auto-ignition)

80517.	Paul, P., and J. Warnatz, "A Re-evaluation of the Means Used to Calculate Transport Properties of Reacting Flows," *Int. Symp. Combust.* 27, 495-504 (1998).	Kinetic Modeling Transport Properties New Approach
80518.	Blasenbrey, T., D. Schmidt and U. Maas, "Automatically Simplified Chemical Kinetics and Molecular Transport and Its Applications in Premixed and Nonpremixed Laminar Flame Calculations," *Int. Symp. Combust.* 27, 505-511 (1998).	Kinetic Modeling Reduced Scheme Chemistry/Transport Implementation
(80194)	Detailed Kinetics, PDF Calculations Method	Turbulent Combustion
80519.	Lindstedt, P., "Modeling of the Chemical Complexities of Flames," *Int. Symp. Combust.* 27, 269-285 (1998).	Laminar Flame Modeling Practical Fuels Species Profiles Review
(80507)	CH_4, C_2H_2, C_2H_4, C_2H_6, NO_x Species Profiles, Measurements, Modeling	CH_3OH/Air
(80195)	Turbulent Combustion, Kinetic Modeling, Reduced Schemes, Gas Turbines, NO_x Predictions	CH_4/Air
80520.	Zhou, X., G. Brenner, T. Weber and F. Durst, "Finite Rate Chemistry in Modeling of Two-Dimensional Jet Premixed CH_4/Air Flame," *Int. J. Heat Mass Transfer* 42, 1757-1773 (1999).	Kinetic Modeling CH_4/Air 2-D Premixed Jet Species Profiles Data Comparisons
80521.	Marinov, N.M., W.J. Pitz, C.K. Westbrook, A.E. Lutz, A.M. Vincitore and S.M. Senkan, "Chemical Kinetic Modeling of a Methane Opposed-Flow Diffusion Flame and Comparison to Experiments," *Int. Symp. Combust.* 27, 605-613 (1998).	Kinetic Modeling CH_4/Air Opposed Flow HC,Aromatic PAH Channels,Profiles
(80151)	Diffusion Flames, Reduced Kinetic Scheme Description	CH_4/Air

80522.	Petersen, E.L., D.F. Davidson and R.K. Hanson, "Kinetics Modeling of Shock Induced Ignition in Low-Dilution CH_4/O_2 Mixtures at High Pressures and Intermediate Temperatures," *Combust. Flame* 117, 272-290 (1999).	Kinetic Modeling CH_4/O_2 Shock Ignited Elevated Pressures
80523.	Sung, C.J., C.K. Law and J.-Y. Chen, "An Augmented Reduced Mechanism for Methane Oxidation with Comprehensive Global Parametric Validation," *Int. Symp. Combust.* 27, 295-304 (1998).	Kinetic Modeling CH_4/O_2 Reduced Scheme Performance
(80344)	Kinetic Modeling, NO_x Control, Reburn Method, Full/Reduced Schemes	CH_4/NH_3
(80500)	Kinetic Modeling, CH, CH_3, CN, NO, LIF/Absorption Monitoring, Comparisons	$CH_4/O_2/NO$
(80337)	Kinetic Modeling, Adequacies, Prompt NO Formation, Temperatures, Species, LIF, Gas Chromatography Monitoring	$CH_4/O_2/N_2$
80524.	D'Anna, A., and A. Violi, "A Kinetic Model for the Formation of Aromatic Hydrocarbons in Premixed Laminar Flames," *Int. Symp. Combust.* 27, 425-433 (1998).	Kinetic Modeling C_2H_4/O_2 Flames Aromatics, PAHS Formation Simulation
80525.	Davis, S.G., C.K. Law and H. Wang, "An Experimental and Kinetic Modeling Study of Propyne Oxidation," *Int. Symp. Combust.* 27, 305-312 (1998).	Kinetic Modeling C_3H_4/O_2 Species Profiles Flow Reactor Data Comparisons
80526.	Klotz, S.D., K. Brezinsky and I. Glassman, "Modeling the Combustion of Toluene/Butane Blends," *Int. Symp. Combust.* 27, 337-344 (1998).	Kinetic Modeling C_4H_{10}/O_2 $C_6H_5CH_3/O_2$ $C_4H_{10}/C_6H_5CH_3/O_2$ Flow Reactor Species Profiles
80527.	Laskin, A., and A. Lifshitz, "Thermal Decomposition of Indene: Experimental Results and Kinetic Modeling," *Int. Symp. Combust.* 27, 313-320 (1998).	Kinetic Modeling C_9H_8/O_2 Product Densities Shock Tube Data/Model Adequacies
(80196)	Turbulent Kinetic/Radiative Submodels, NO Formation	$H_2/O_2/He$
(80334)	Gas Turbines, Fuel 'N', Kinetic Modeling	NO_x Formation

80528. Sendt, K., E. Ikeda, G.B. Bacskay and J.C. Mackie, "Ab Initio Quantum Chemical and Experimental (Shock Tube) Studies of the Pyrolysis Kinetics of Acetonitrile," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1054-1072 (1999).

Pyrolysis
CH_3CN/Ar
Rate Constants
Products
Shock Tube
Kinetic Modeling
$\Delta H_f(CH_2CN)$

(80371) Pyrolysis, C_n Nanotubes Formation

C_2H_2/$Fe(CO)_5$/Ar

80529. Hynes, R.G., J.C. Mackie and A.R. Masri, "Shock Tube Study of the Pyrolysis of the Halon Replacement Molecule CF_3CHFCF_3," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 54-61 (1999).

Pyrolysis
CF_3CHFCF_3/Ar
Product Yields
Kinetic Modeling
Rate Constants

80530. Choudhary, V.R., V.H. Rane and A.M. Rajput, "Simultaneous Thermal Cracking and Oxidation of Propane to Propylene and Ethylene," *AIChE J.* 44, 2293-2301 (1998).

Pyrolysis
C_3H_8/O_2/Steam
Thermal Cracking
C_2H_4, C_3H_6
Product Yields

80531. Hore, N.R., and D.K. Russell, "Radical Pathways in the Thermal Decomposition of Pyridine and Diazines: A Laser Pyrolysis and Semiempirical Study," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 269-275 (1998).

IR Laser Pyrolysis
c-C_5H_5N/SF_6
c-$C_4H_4N_2$/SF_6
Product FTIR
Mechanisms

80532. Roy, K., C. Horn, P. Frank, V.G. Slutsky and T. Just, "High Temperature Investigations on the Pyrolysis of Cyclopentadiene," *Int. Symp. Combust.* 27, 329-336 (1998).

Pyrolysis
c-C_5H_6 + Ar
c-C_5H_5 + Ar
Rate Constants
Shock Tube
Kinetic Model

80533. Kern, R.D., Q. Zhang, J. Yao, B.S. Jursic, R.S. Tranter, M.A. Greybill and J.H. Kiefer, "Pyrolysis of Cyclopentadiene: Rates for Initial C-H Bond Fission and the Decomposition of *c*-C_5H_5," *Int. Symp. Combust.* 27, 143-150 (1998).

Pyrolysis
c-C_5H_6 + Ne
c-C_5H_5 + Ne
Rate Constants
RRKM Analysis
Shock Tube
ΔH_f(c-C_5H_5)

80534. Horn, C., K. Roy, P. Frank and T. Just, "Shock Tube Study on the High Temperature Pyrolysis of Phenol," *Int. Symp. Combust.* 27, 321-328 (1998).

Pyrolysis
C_6H_5OH
C_6H_5OH + H
Rate Constants
Branching Ratio
Shock Tube
Kinetic Modeling

(80079) Pyrolysis, Product Oil PAH Content, Steam Effects — Oil Shales

(80078) Yields of Char and Activated Carbons, Properties — Tire Pyrolysis

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

80535. Belouaggadia, N., and R. Brun, "Chemical Rate Constants in Nonequilibrium Flows," Presented Originally as AIAA Paper 97-2555 at the *32nd AIAA Thermophysics Conference*, Held in Atlanta GA, June 1997, *J. Thermophys. Heat Transfer* 12, 482-488 (1998).

Rate Constants
Nonequilibrium
Diatomic Flows
Vibrational Effects

80536. Fontijn, A., "Wide Temperature Range Observations on Reactions of Metal Atoms and Small Radicals," *Pure Appl. Chem.* 70, 469-476 (1998).

$AlCl + CO_2, O_2$
$BCl + CO_2, O_2$
$Metals + N_2O$
Rate Constants
T Dependences
Overview

80537. Belyung, D.P., G.T. Dalakos, J.-D.R. Rocha and A. Fontijn, "Wide Temperature Range Kinetics of the BO Reactions with O_2, HCl and CO_2: Comparison to AlO Reactions," *Int. Symp. Combust.* 27, 227-233 (1998).

$BO + CO_2$
$BO + HCl, O_2$
Rate Constants
T Dependences
Measurements

80538. Aranda, A., G. Laverdet, G. Le Bras and G. Poulet, "Kinetic Study of the $CH_3O_2 + Br$ Reaction at 298 K," *J. de Chim. Phys.* 95, 963-972 (1998).

$Br + CH_3O_2$
Rate Constant

80539. Bedjanian, Y., G. Le Bras and G. Poulet, "Kinetics and Mechanism of the $IO + BrO$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10501-10511 (1998).

$BrO + IO$
Branching Ratios
$BrO + BrO$
BrO,IO/Wall
$BrO + IBr, I_2$
$Br + IO$
$I, NO + O_3$
Rate Constants
$\Delta H_f(IO_2)$

80540. Li, Z., "Laboratory Formation of OBrO and Its Reactivity Toward Ozone at 298 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1206-1213 (1999).

$BrO_2 + O_3$
$BrO_2(v) + O_3$
Rate Constants
Measurements

80541. Costes, M., and C. Naulin, "State-to-State Cross Sections for the $C(^3P_J)+O_2(X^3\Sigma_g^-)\rightarrow CO(X^1\Sigma^+)+O(^1D_2)$ Reaction at Kinetic Energies Between 4.4 and 90 meV," *Compt. Rendus Acad. Sci. Paris, Ser. II, Part c. Chimie* 1, 771-775 (1998).

$C+O_2$
Cross Sections
4.4-90 meV
CO(v=15-17)
Product

80542. Yuan, J., L. Wells and P. Marshall, "Kinetic Studies of the Reaction of Atomic Hydrogen with Trifluoroiodomethane," *Chem. Phys. Lett.* 297, 553-557 (1998).

CF_3I+H
Rate Constants
T Dependence

80543. Kumaran, S.S., J.J. Carroll and J.V. Michael, "The Branching Ratio in the Thermal Decomposition of H_2CO," *Int. Symp. Combust.* 27, 125-133 (1998).

HCHO+Kr
Rate Constants
Branching Ratio
Measurements
RRKM
Comparisons

80544. Fittschen, C., B. Delcroix, N. Gomez and P. Devolder, "Rate Constants for the Reactions of CH_3O with CH_2O, CH_3CHO and *i*-C_4H_{10}," *J. de Chim. Phys.* 95, 2129-2142 (1998).

CH_3O+CH_2O
CH_3O+CH_3CHO
CH_3O+*i*-C_4H_{10}
Rate Constants
T,P Dependences

80545. Troe, J., "Modeling the Temperature and Pressure Dependence of the Reaction $HO+CO\leftrightarrow HOCO\leftrightarrow H+CO_2$," *Int. Symp. Combust.* 27, 167-175 (1998).

CO+OH
Rate Constants
RRKM Data Fitting
High/Low Pressure
Expressions

80546. Eremin, A.V., D. Woiki and P. Roth, "Measurement of $O(^1D)$ Formation During Thermal Decomposition of CO_2 Behind Shock Waves," *Shock Waves* 6, 79-83 (1996).

CO_2+Ar
$O(^1D)$ Product
Channel
Rate Constant
Shock Tube

80547. Kruse, T., and P. Roth, "High Temperature Reactions of C_2 with Atomic and Molecular Oxygen," *Int. Symp. Combust.* 27, 193-200 (1998).

C_2+O
C_2+O_2
Rate Constants
T Dependences
Shock Tube

80548. Hoobler, R.J., and S.R. Leone, "Low Temperature Rate Coefficients for Reactions of the Ethynyl Radical (C_2H) with C_3H_4 Isomers Methylacetylene and Allene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1342-1346 (1999).

$C_2H+C_3H_4$
Rate Constants
Isomeric Effects
T Dependences

80549. Miller, J.A., J.L. Durant and P. Glarborg, "Some Chemical Kinetics Issues in Reburning: The Branching Fraction of the HCCO+NO Reaction," *Int. Symp. Combust.* 27, 235-243 (1998).

CHCO+NO
HCNO+O,OH
Rate Constants
Branching Ratio
Calculations

80550. Hranisavljevic, J., S.S. Kumaran and J.V. Michael, "$H + CH_2CO \rightarrow CH_3 + CO$ at High Temperature: A High Pressure Chemical Activation Reaction with Positive Barrier," *Int. Symp. Combust.* 27, 159-166 (1998).

$CH_2CO + H$
Rate Constants
T Dependence
Shock Tube

(80528) Rate Constants, Shock Tube Pyrolysis, Products, $\Delta H_f(CH_2CN)$, Kinetic Modeling

CH_3CN/Ar

80551. Crawford, M.A., T.J. Wallington, J.J. Szente, M.M. Maricq and J.S. Francisco, "Kinetics and Mechanism of the Acetylperoxy + HO_2 Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 365-378 (1999).

$CH_3C(O)O_2 + HO_2$
$CH_3C(O)OH + Cl$
$CH_3C(O)OOH + Cl$
Rate Constants
Mechanisms

80552. Miyokawa, K., and E. Tschuikow-Roux, "Kinetics of the Photobromination of Dichloro- and Dibromoethane: Estimate of the C-H Bond Dissociation Energies and the Heats of Formation of the CH_3CCl_2 and CH_3CBr_2 Radicals," *Bull. Chem. Soc. Jpn .* 72, 1-5 (1999).

$C_2H_4Cl_2 + Br$
$C_2H_4Br_2 + Br$
α-H Abstraction
Rate Constants
T Dependences
$\Delta H_f(CH_3CCl_2)$
$\Delta H_f(CH_3CBr_2)$

80553. Urbanski, S.P., R.E. Stickel and P.H. Wine, "Mechanistic and Kinetic Study of Gas Phase Reaction of Hydroxyl Radical with Dimethyl Sulfoxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10522-10529 (1998).

$(CH_3)_2SO + OH$
Rate Constant
CH_3 Product Yield
Mechanism

80554. Denisov, E.T., "The Reactivity of Ketyl and Alkyl Radicals in Reactions with Carbonyl Compounds," *Russ. Chem. Bull.* 47, 2110-2116 (1998).

$R_1R_2COH + R_3COR_4$
$R_5 + R_3COR_4$
H-Atom Transfer
Activation Energies
Trends,Model

(80529) Rate Constants, Shock Tube Pyrolysis, Product Yields, Kinetic Modeling

CF_3CHFCF_3/Ar

80555. DeMore, W.B., and E.W. Wilson Jr, "Rate Constant and Temperature Dependence for the Reaction of Hydroxyl Radicals with 2-Fluoropropane (HFC-281ea)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 573-576 (1999).

$C_3H_7F + OH$
Rate Constants
Temperature Dependence

(80532) Rate Constants, Shock Tube Pyrolysis, Kinetic Modeling

c-C_5H_6 + Ar
C_5H_5 + Ar

(80533) Rate Constants, Shock Tube Pyrolysis, RRKM Analysis, ΔH_f (*c*-C_5H_5)

c-C_5H_6 + Ne
c-C_5H_5 + Ne

80556. Tsang, W., J.A. Walker and J.A. Manion, "Single Pulse Shock Tube Study on the Decomposition of 1-Pentyl Radicals," *Int. Symp. Combust.* 27, 135-142 (1998).

1-$C_5H_{11}\rightarrow$
1-$C_5H_{11}I\rightarrow$
Dissociation
Rate Constants
Branching Ratios
Shock Tube

80557. Van Der Loos, A., J. Vandooren and P.J. Van Tiggelen, "Kinetic Study of Methyl *tert*-Butyl Ether (MTBE) Oxidation in Flames," *Int. Symp. Combust.* 27, 477-484 (1998).

t-$C_4H_9OCH_3+O,H$
t-$C_4H_9OCH_3+OH$
Rate Constants
$H_2/C_4H_9OCH_3/O_2$
Flame Sampling
Species Profile

80558. Wallington, T.J., H. Egsgaard, O.J. Nielsen, J. Platz, J. Sehested and T. Stein, "Ultraviolet-Visible Spectrum of the Phenyl Radical and Kinetics of Its Reaction with NO in the Gas Phase," *Chem. Phys. Lett.* 290, 363-370 (1998).

C_6H_5+NO
Rate Constant
C_6H_5 UV Absorption
Cross Sections

(80534) Rate Constants, Shock Tube Pyrolysis, Branching Ratio, Kinetic Modeling

$C_6H_5OH\rightarrow$
C_6H_5OH+H

80559. Eng, R.A., C. Fittschen, A. Gebert, P. Hibomvschi, H. Hippler and A.-N. Unterreiner, "Kinetic Investigations of the Reactions of Toluene and of *p*-Xylene with Molecular Oxygen Between 1050 and 1400 K," *Int. Symp. Combust.* 27, 211-218 (1998).

$C_6H_5CH_3+HO_2,O_2$
$C_6H_4(CH_3)_2+O_2$
$CH_3C_6H_4CH_2+O_2$
Rate Constants
Shock Tube

80560. Becker, K.H., C. Dinis, H. Geiger and P. Wiesen, "Kinetics of the Reaction of OH with di-*n*-Butoxymethane in the Range 298-710 K," *Chem. Phys. Lett.* 300, 460-464 (1999).

$CH_2(OC_4H_9)_2+OH$
Rate Constant
Measurement

80561. Mellouki, A., "Kinetic Studies of Cl Atom Reactions with Series of Alkanes Using the Pulsed Laser Photolysis-Resonance Fluorescence Method," *J. de Chim. Phys.* 95, 513-522 (1998).

$Cl+CH_4,C_2H_6$
$Cl+C_3H_8,C_4H_{10}$
Rate Constants

80562. Fantechi, G., N.R. Jensen, O. Saastad, J. Hjorth and J. Peeters, "Reactions of Cl Atoms with Selected Volatile Organic Compounds (VOCs): Kinetics, Products and Mechanisms," *J. Atm. Chem.* 31, 247-267 (1998).

$Cl+C_5H_8$
$Cl+C_6H_5CH_3$
Rate Constants
$Cl+C_5H_9OH$
Major Products

80563. Sokolov, O., M.D. Hurley, T.J. Wallington, E.W. Kaiser, J. Platz, O.J. Nielsen, F. Berho, M.-T. Rayez and R. Lesclaux, "Kinetics and Mechanism of the Gas Phase Reaction of Cl Atoms with Benzene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10671-10681 (1998).

$Cl+C_6H_6$
$C_6H_6.Cl+O_2$
$Cl+CHF_2Cl$
Rate Constants
Channels

(80607) Cross Sections, 1 eV Energy, $Cl(^2P_{1/2,3/2})$ Product Energies

Hot 'H' + HCl

80564. Mueller, M.A., R.A. Yetter and F.L. Dryer, "Measurement of the Rate Constant for $H+O_2+M \rightarrow HO_2+M$ ($M=N_2$,Ar) Using Kinetic Modeling of the High Pressure $H_2/O_2/NO_x$ Reaction," *Int. Symp. Combust.* 27, 177-184 (1998).

$H+O_2+Ar(N_2)$
Rate Constants
$H_2/O_2/NO$
Flow Reactor
Modeling

80565. Ashman, P.J., and B.S. Haynes, "Rate Coefficient of $H+O_2+M \rightarrow HO_2+M$ ($M=H_2O,N_2,Ar,CO_2$)," *Int. Symp. Combust.* 27, 185-191 (1998).

$H+O_2+M$
Rate Constants
$M=Ar,CO_2,H_2O,N_2$
$H_2/O_2/NO$
Flow Reactor
Modeling

80566. Schading, G.N., and P. Roth, "Sublimation and Dissociation of Cyanuric Acid Particles and Dissociation of Isocyanic Acid Vapor," *Int. Symp. Combust.* 27, 245-251 (1998).

$HNCO+Ar$
$(HNCO)_3 \rightarrow$
Rate Constants
CO,OH Channels
Shock Tube

80567. Glarborg, P., M. Ostberg, M.U. Alzueta, K. Dam-Johansen and J.A. Miller, "The Recombination of Hydrogen Atoms with Nitric Oxide at High Temperatures," *Int. Symp. Combust.* 27, 219-226 (1998).

$NO+H+N_2$
Rate Constants
T Dependence
$CO/O_2/H_2O/N_2$
Flow Reactor

80568. Gierczak, T., J.B. Burkholder and A.R. Ravishankara, "Temperature Dependent Rate Coefficient for the Reaction $O(^3P)+NO_2 \rightarrow NO+O_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 877-883 (1999).

NO_2+O
Rate Constant
UV Absorption
Cross Section
T Dependences

80569. McClean, R.E., "Depletion Kinetics of Nickel Atoms by Sulfur Dioxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 75-79 (1999).

$Ni+SO_2+Ar$
$Ni(a^3D_J)+SO_2+Ar$
Rate Constants
$D(NiSO_2)$
Measurements

(80815) Reactive Channel/Vibrational Relaxation, Branching Ratios, Rate Constants, Measurements

$OH(v=1,2)+CH_4$

80570. Pfeiffer, T., O. Forberich and F.J. Comes, "Tropospheric OH Formation by Ozonolysis of Terpenes," *Chem. Phys. Lett.* 298, 351-358 (1998).

O_3+Terpenes
Rate Constants
7 Molecules
OH Product
Yields

80571. Garland, N.L., "Temperature Dependence of the Reaction: $SO+O_2$," *Chem. Phys. Lett.* 290, 385-390 (1998).

$SO+O_2$
Rate Constants
Temperature
Dependence
Measurements

80572. Kunz, A., and P. Roth, "Dissociation of $SiCl_4$ Based on Cl- and Si-Concentration Measurements," *Int. Symp. Combust.* 27, 261-267 (1998).

$SiCl_4$+Ar
SiCl+Ar
Rate Constants
Shock Tube

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

80573. Rakitzis, T.P., and R.N. Zare, "Photofragment Angular Momentum Distributions in the Molecular Frame: Determination and Interpretation," *J. Chem. Phys.* 110, 3341-3350 (1999).

AB+hν
Photofragment
Angular
Momenta/
Polarization
Theory

80574. Herwig, A., M. Braun and V. Engel, "Structures in Molecular Photofragment and Photoelectron Distributions from Two-Photon Non-Resonant Excitation," *Chem. Phys. Lett.* 300, 269-274 (1999).

2-Photon (Color)
Dissociation
Resonant/
Non Resonant
Differences
Calculations

80575. Cao, J., H. Ihee and A.H. Zewail, "Ultrafast Electron Diffraction: Determination of Radical Structure with Picosecond Time Resolution," *Chem. Phys. Lett.* 290, 1-8 (1998).

CF_2I_2+hν
ps Time Resolution
Product CF_2
Electron Diffraction
Structure Monitor

80576. Clark, R.J.H., J.R. Dann and L.J. Foley, "Matrix Isolation Study of the Photochemically Induced Reaction of Ozone with Dibromochloromethane and Bromodichloromethane in Solid Argon at 14 K: FTIR Spectra of the Complexes C(O)HCl··BrX, C(O)HBr··XCl, C(O)BrCl··HX, (OC)(HCl)(Br_2), (OC)(HBr)(Cl_2), and (OC)(BrCl)(HX) (where X=Br or Cl)," *J. Chem. Soc., Dalton Trans.* 73-78 (1999).

$CHClBr_2/O_3$+hν
$CHCl_2Br/O_3$+hν
Product FTIR
Matrix Study

80577. Petrov, A.K., E.N. Chesnokov, S.R. Gorelik, K.D. Straub, E.B. Szarmes and J.M.J. Madey, "^{15}N Isotope-Selective Infrared Multiphoton Dissociation of Nitromethane by a Free Electron Laser," *Russ. Chem. Bull.* 47, 719-722 (1998).

IR MPD
CH_3NO_2
^{15}N Isotope
Selectivity
1400-1550 cm^{-1}

80578. Bise, R.T., H. Choi, H.B. Pedersen, D.H. Mordaunt and D.M. Neumark, "Photodissociation Spectroscopy and Dynamics of the Methylthio Radical, CH_3S," *J. Chem. Phys.* 110, 805-816 (1999).

CH_3S+hν
CD_3S+hν
(A-X) Dissociation
$CH_3(v),S(^3P_J)$
Product Distributions
$\Delta H_f(CH_3S)$
Predissociation

80579. Lin, J.J., T.C. Hsu, D.W. Hwang, Y.T. Lee and X. Yang, "Photodissociation Dynamics of Trifluoroethylene at 157 nm Excitation," *J. Chem. Phys.* 109, 10719-10726 (1998).

$CF_2CHF + h\nu$
Product
Kinetic Energies
4 Channels
Branching Ratios
Energy Partitioning

80580. Lin, J.J., S.M. Wu, D.W. Hwang, Y.T. Lee and X. Yang, "Photodissociation Dynamics of 1,1-Difluoroethylene at 157 nm Excitation," *J. Chem. Phys.* 109, 10838-10846 (1998).

$C_2H_2F_2 + h\nu$
5 Channels
Product
Kinetic Energies
Dynamics

80581. Cattaneo, P., and M. Persico, "Semiclassical Treatment of the Photofragmentation of Azomethane," *Chem. Phys. Lett.* 289, 160-166 (1998).

$(CH_3)_2N_2 + h\nu$
Photodissociation
Dynamics
Calculations

80582. Ni, C.-K., J.D. Huang, Y.T. Chen, A.H. Kung and W.M. Jackson, "Photodissociation of Propyne and Allene at 193 nm with Vacuum Ultraviolet Detection of the Products," *J. Chem. Phys.* 110, 3320-3325 (1999).

$C_3H_4 + h\nu$
Channels
Product Monitoring
Isomeric Effects

80583. Deyerl, H.-J., I. Fischer and P. Chen, "Photodissociation Dynamics of the Allyl Radical," *J. Chem. Phys.* 110, 1450-1462 (1999).

$C_3H_5 + h\nu$
Channels
Branching Ratios
Energies
Measurements

80584. Castillejo, M., S. Couris, E. Koudoumas and M. Martin, "Subpicosecond Ionization and Dissociation of Benzene and Cyclic Alkanes at 800 and 400 nm," *Chem. Phys. Lett.* 289, 303-310 (1998).

fs MPD/MPI
c-C_3H_6, C_6H_6
c-C_6H_{12}
Product Ions
Fragmentations

80585. Kessler, A., U. Kensy and B. Dick, "NO Product Yield Excitation Spectrum of the ($S_0 \rightarrow S_2$) Transition of Nitrosobenzene in a Supersonic Jet," *Chem. Phys. Lett.* 289, 516-520 (1998).

$C_6H_5NO(S_2\text{-}S_0)$
Excitation
NO Fragment
Yield
S_2 Lifetime

(80493) Laser Photolysis, Product NO LIF Monitoring Method, Sensitivity

$C_6H_5NO_2 + h\nu$

80586. Hansen, K., R. Muller and E.E.B. Campbell, "Comment on the Photofragmentation of C_{60} in Seeded Supersonic Molecular Beams: Effects of Rovibrational Cooling," *Chem. Phys. Lett.* 301, 105-108 (1999).

C_{60}
Photofragment
Mass Spectra
Anomalies
Cluster Effects

80587. Biasioli, F., A. Boschetti, P. Piseri, P. Milani and S. Iannotta, "Reply to the Comment on the Photofragmentation of C_{60} in Seeded Supersonic Molecular Beams: Effects of Rovibrational Cooling," *Chem. Phys. Lett.* 301, 109-111 (1999).

Reply

80588. Kreher, C.J., R.T. Carter and J.R. Huber, "Photodissociation of OClO and Ar/OClO and H_2O/OClO Clusters Studied by the Resonance Enhanced Multiphoton Ionization-Time-of-Flight Method," *J. Chem. Phys.* 110, 3309-3319 (1999).

$ClO_2 + h\nu$
$(ClO_2)_n + h\nu$
$ClO_2Ar_n + h\nu$
$ClO_2(H_2O)_n + h\nu$
Product
ClO,O
Energies

80589. Bartz, J.A., T.O. Friday, B.R. Goodman, S.E. Kooi, R.G. Blair and W.F. Polik, "Energy Disposal in the Photodissociation of $Co(CO)_3NO$ Near 225 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10697-10702 (1998).

$Co(CO)_3NO + h\nu$
Co*,NO(J)
Product
Distributions

80590. Rubner, O., and V. Engel, "Fragmentation Dynamics of $Fe(CO)_5$ Upon Femtosecond Excitation: A Time-Dependent Statistical Description," *Chem. Phys. Lett.* 293, 485-490 (1998).

fs MPD
$Fe(CO)_5$
Fragmentation
Modeling

(80744) Photodissociation Dynamics, P.E. Surface, Calculations

$H_2O(A).Ar_n$

80591. Luckhaus, D., J.L. Scott and F.F. Crim, "An Experimental and Theoretical Study of the Vibrationally Mediated Photodissociation of Hydroxylamine," *J. Chem. Phys.* 110, 1533-1541 (1999).

$NH_2OH(4,5\nu_{OH}) + h\nu$
Energies < 42000 cm^{-1}
NH_2,OH(v,J)
Product Energies
Dynamics

80592. Maas, D.J., D.I. Duncan, R.B. Vrijen, W.J. van der Zande and L.D. Noordam, "Vibrational Ladder Climbing in NO by (sub)Picosecond Frequency-Chirped Infrared Laser Pulses," *Chem. Phys. Lett.* 290, 75-80 (1998).

ps IR MPA
NO
Vibrational
Ladder Climbing
v=1-3

80593. Zeiri, Y., G. Katz, R. Kosloff, M.S. Topaler, D.G. Truhlar and J.C. Polanyi, "Quantum Mechanism in the Photodissociation of NaFH Complex: A Challenge to Semiclassical Analysis," *Chem. Phys. Lett.* 300, 523-528 (1999).

Na.HF + hν
Dynamics
Calculations
Theoretical
Difficulties

80594. Davidsson, J., T. Hansson and E. Mukhtar, "Ultrafast Multiphoton Ionization Dynamics and Control of NaK Molecules," *J. Chem. Phys.* 109, 10740-10753 (1998).

MPI
NaK
fs Pump/Probe
NaK^+,Na^+
Channels
P.E. Curves
Pathway Control

80595. Lacoursiere, J., S.A. Meyer, G.W. Faris, T.G. Slanger, B.R. Lewis and S.T. Gibson, "The $O(^1D)$ Yield from O_2 Photodissociation Near H Lyman-α (121.6 nm)," *J. Chem. Phys.* 110, 1949-1958 (1999).

$O_2 + h\nu$(121.6 nm)
$O(^1D)$ Yields
T Dependence
Isotope Effects

80596. O'Keeffe, P., T. Ridley, S. Wang, K.P. Lawley and R.J. Donovan, "Photodissociation of Ozone Between 335 and 352 nm to Give $O_2(b^1\Sigma_g^+) + O(^3P_J)$," *Chem. Phys. Lett.* 298, 368-374 (1998).

$O_3 + h\nu$
335-352 nm
Spin Forbidden
Channel
Observation

80597. Kunz, A., and P. Roth, "Laser Flash Photolysis of $SiCl_4$ at High Temperatures Based on Si and Cl Concentration Measurements," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 841-846 (1999).

$SiCl_4 + h\nu$
High Temperatures
Si,Cl Absorption
Monitoring
Kinetic Model

80598. Tada, N., K. Tonokura, K. Matsumoto, M. Koshi, A. Miyoshi and H. Matsui, "Photolysis of Disilane at 193 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 322-329 (1999).

$Si_2H_6 + h\nu$
Channels
H, SiH_2, Si_3H_8
Product
Quantum Yields

(80877) Photodissociation Measurements, D

W $C_2H_2^+ + h\nu$

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

80599. Blokhin, A.P., M.F. Gelin, I.I. Kalosha, S.A. Polubisok and V.A. Tolkachev, "Polarized Fluorescence of Polyatomic Fragments Produced Through Photodissociation of Polyatomic Molecules in the Gas Phase," *J. Chem. Phys.* 110, 978-993 (1999).

Polarized
Product Emission
$ABC + h\nu$
Polyatomics
Theory

(80621) Product Energies, Unimolecular Dissociation, Exit Channel Dynamics

$ABC/AB + C$

80600. Zhang, H., R.-s. Zhu, G.-J. Wang, K.-L. Han, G.-Z. He and N.-Q. Lou, "Photofragment Translational Spectroscopy of *p*-Bromotoluene at 266 nm," *Chem. Phys. Lett.* 300, 483-488 (1999).

$Br(^2P_{1/2,3/2})$
Photofragment
Kinetic Energies
Anisotropy
$BrC_6H_4CH_3 + h\nu$

80601. Zhang, H., R.-S. Zhu, G.-J. Wang, K.-L. Han, G.-Z. He and N.-Q. Lou, "Photodissociation of Bromobenzene at 266 nm," *J. Chem. Phys.* 110, 2922- 2927 (1999).

Br
Product Energies
Anisotropy
$C_6H_5Br + h\nu$
Mechanism

80602. Regan, P.M., S.R. Langford, A.J. Orr-Ewing and M.N.R. Ashfold, "The Ultraviolet Photodissociation Dynamics of Hydrogen Bromide," *J. Chem. Phys.* 110, 281-288 (1999).

$Br(^2P_{1/2,3/2})$
Branching Ratios
Recoil Anisotropies
$HBr + h\nu$

(80436) Br_2(B).He, v=10, 39-48, Predissociation, Product Distributions, Measurements

Br_2(B,v,J)

80603. Kaiser, R.I., C. Ochsenfeld, M. Head-Gordon and Y.T. Lee, "Crossed-Beam Reaction of Carbon Atoms with Sulfur Containing Molecules. I. Chemical Dynamics of Thioformyl (HCS X^2A') Formation from Reaction of $C(^3P_j)$ with Hydrogen Sulfide, $H_2S(X^1A_1)$," *J. Chem. Phys.* 110, 2391-2403 (1999).

HCS Product Angular Distributions
$C + H_2S$
Crossed Beams Dynamics

80604. Eppink, A.T.J.B., and D.H. Parker, "Energy Partitioning Following Photodissociation of Methyl Iodide in the A-Band: A Velocity Mapping Study," *J. Chem. Phys.* 110, 832-844 (1999).

CH_3(T,v,J)
$I(^2P_{1/2,3/2})$
Product Energies
2-D Imaging
$CH_3I + h\nu$
Dynamics
$D(CH_3I)$

(80541) Product Distribution, $C + O_2$ Cross Sections, 4.4-90 meV Energy

CO(v=15-17)

(80241) Product Vibrational Distributions, $CO_2^+ + C_6F_6^-$ Neutralization, Spectral Emission

CO(d,a′)

80605. Zyrianov, M., T. Droz-Georget and H. Reisler, "Fragment Recoil Anisotropies in the Photoinitiated Decomposition of HNCO," *J. Chem. Phys.* 110, 2059-2068 (1999).

CO,H,NH
Product Recoil Anisotropies
$HNCO + h\nu$
3 Channels Dynamics

(80635) Atom Product Energies, $C_6H_5X^+$, Unimolecular Dissociation, X=Cl,Br,I, Measurements

Cl,Br,I

80606. Rakitzis, T.P., S.A. Kandel, A.J. Alexander, Z.H. Kim and R.N. Zare, "Measurements of Cl-Atom Photofragment Angular Momentum Distributions in the Photodissociation of Cl_2 and ICl," *J. Chem. Phys.* 110, 3351-3359 (1999).

Cl
Product Angular Momenta
$Cl_2 + h\nu$
$ICl + h\nu$
Single/Multiple Surface Formalism

80607. Brownsword, R.A., C. Kappel, P. Schmiechen, H.P. Upadhyaya and H.-R. Volpp, "Dynamics of the H+HCl Gas Phase Reaction: Absolute Reactive Cross Section for $Cl(^2P_{3/2})$ Atom Formation," *Chem. Phys. Lett.* 289, 241-246 (1998).

$Cl(^2P_{1/2,3/2})$
Product Energies
'Hot' H+HCl
1 eV Energy
Cross Sections

80608. Baumgartel, S., R.F. Delmdahl, K.-H. Gericke and A. Tribukait, "Reaction Dynamics of $Cl+O_3 \rightarrow ClO+O_2$," *Eur. Phys. J. D* 4, 199-205 (1998).

ClO(v,J,Λ)
Product Distributions
$Cl+O_3$
Vibrational Relaxation
$ClO(v)+N_2$
Rate Constant

(80441) Product States, $Cl_2(B,v)$.Ne Predissociation, Lifetimes, Calculations

$Cl_2(B)$

(80442) $Cs(6^2D_{3/2})+H_2$ Reactive Quenching Cross Sections, Product Distributions, Measurements

CsH(v,J)

80609. Ahmed, M., D.S. Peterka and A.G. Suits, "Crossed Beam Reaction of $O(^1D)+D_2 \rightarrow OD+D$ by Velocity Map Imaging," *Chem. Phys. Lett.* 301, 372-378 (1999).

D Product
Velocity Mapping
$O(^1D)+D_2$
Crossed Beams

80610. Chapman, W.B., B.W. Blackmon, S. Nizkorodov and D.J. Nesbitt, "Quantum State-Resolved Reactive Scattering of $F+H_2$ in Supersonic Jets: Nascent HF(v,J) Rovibrational Distributions via Infrared Laser Direct Absorption Methods," *J. Chem. Phys.* 109, 9306-9317 (1998).

HF(v,J)
Product Energy Distributions
$F+H_2$
Measurements

80611. Tsuji, M., M. Nakamura, Y. Nishimura, E. Oda, H. Oota and M. Hisano, "Formation of He* by Ion-Ion Neutralization Reactions of He^+ with $C_6F_5X^-$ (X=F,Cl,Br,CF_3) in a Helium Flowing Afterglow," *J. Chem. Phys.* 110, 2903-2910 (1999).

He*
Rydberg State Distributions
$He^+ + C_6F_5X^-$
X=F,Cl,Br,CF_3
Measurements
Modeling

80612. Li, H., K.J. Franks and W. Kong, "Photodissociation of ICN in a Brute-Force Field: Detection of the ($I^2P_{1/2}$) Product," *Chem. Phys. Lett.* 300, 247-252 (1999).

$I(^2P_{1/2})$
Product
ICN + hν
Orientation Effects

(80448) $N(^2D)+H_2O/D_2O$, Channels, Product Energies

NH(v,J),OH(v,J)
H,D Energies

(80252) $NO^+(v)+C_6F_6^-$ Neutralization, Product Distribution, Spectral Emission, Reactant Vibrational Effects

NO(D,C,A)

80613. Mo, Y., H. Katayanagi and T. Suzuki, "Probing the Alignment of $NO(X^2\Pi)$ by [2+1] Resonance Enhanced Multiphoton Ionization via the $C^2\Pi$ State: A Test of Semiclassical Theory in 355 nm Photodissociation of NO_2," *J. Chem. Phys.* 110, 2029-2041 (1999).

NO(X,v,J)
Product Vector Correlations
NO_2 + hν
2-D Imaging
Data/Theory Comparisons

80614. Neyer, D.W., A.J.R. Heck and D.W. Chandler, "Photodissociation of N_2O: J-Dependent Anisotropy Revealed in N_2 Photofragment Images," *J. Chem. Phys.* 110, 3411-3417 (1999).

$N_2(v=0,J=40\text{-}90)$
Photofragment Anisotropies
$N_2O+h\nu$
REMPI Probe
$N_2(v=1)$ Detection

(80254) Product Distribution, $Ne(^3P_{0,2})+N_2$ Penning Ionization, Well Depth, $N_2^+(A)$ Intermediate

$N_2^+(v)$

(80453) Product Branching Ratios, OH(A,v,N) Predissociation Rates, Calculations

$O(^3P_J)$

80615. Blunt, D.A., and A.G. Suits, "Photodissociation of Ozone at 276 nm by Photofragment Imaging and High Resolution Photofragment Translational Spectroscopy," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 99-106 (1997).

$O(^1D),O_2(a,v)$
Product Distributions
Alignments
$O_3+h\nu(276\text{ nm})$
REMPI,TOF

(80374) Product Energies, $H_2.OH(2\nu_{OH})$ Half Collision Predissociation Reaction, IR Pump/UV Probe

$OH(v=1,J)$

80616. Fan, L.-H., J.-J. Chen, Y.-Y. Lin and W.-T. Luh, "Reaction of $Rb(5^2D,7^2S)$ with H_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1300-1305 (1999).

RbH(T,v,J)
Product Energy Distributions
$Rb(5^2D,7^2S)+H_2$
Measurements

80617. Hansen, N., U. Andresen, H. Dreizler, J.-U. Grabow, H. Mader and F. Temps, "Fourier Transform Microwave Observation of $SO(X^3\Sigma,v=0\text{-}2)$ Produced by 193 nm Photodissociation of SO_2 in a Pulsed Supersonic Jet Expansion," *Chem. Phys. Lett.* 289, 311-318 (1998).

$SO(X,v=0\text{-}2)$
Product
$SO_2+h\nu$
Jet Expansion

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

80618. Hase, W.L., "Some Recent Advances and Remaining Questions Regarding Unimolecular Rate Theory," *Acc. Chem. Res.* 31, 659-665 (1998).

Unimolecular Reaction Rate Theory
Status Review

80619. Kiefer, J.H., "Some Unusual Aspects of Unimolecular Falloff of Importance in Combustion Modeling," *Int. Symp. Combust.* 27, 113-124 (1998).

Unimolecular Fall-off
RRKM Theory
Combustion
Kinetic Modeling
Difficulties

80620.	Gershinsky, G., and B.J. Berne, "The Dependence of the Rate Constant for Isomerization on the Competition Between Intramolecular Vibrational Relaxation and Energy Transfer to the Bath: A Stochastic Model," *J. Chem. Phys.* 110, 1053-1060 (1999).	Unimolecular Isomerization IVR Effects Model
80621.	Bonnet, L., and J.C. Rayez, "On the Analysis of Exit-Channel Effects in Three -Atom Unimolecular Reactions," *Eur. Phys. J. D* 4, 169-179 (1998).	Unimolecular Dissociation ABC/AB+C Product Energies Exit Channel Dynamics
80622.	Martins, L.M.M.de A., G. Arbilla and E.C. da Silva, "Unimolecular Decomposition of Formaldehyde: $H_2CO \rightarrow H_2+CO$. I. Ab Initio Reaction Path and Variational Transition State Rate Constants," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10805-10812 (1998).	Unimolecular Dissociation CH_2O Rate Constants Reaction Path Calculations
80623.	Wang, B., H. Hou and Y. Gu, "Features of the Potential Energy Surface for the Decomposition of CH_3OF," *Chem. Phys. Lett.* 300, 99-103 (1999).	Unimolecular Dissociation CH_3OF P.E. Surface Channels Energies
(80807)	Isomerization, -CH_2(F) Stretch, IVR, Lifetime, Measurements	CH_2FCH_2OH
80624.	Stanton, J.F., and J. Guass, "An Estimation of the Isomerization Energy of Acetylene," *J. Chem. Phys.* 110, 1831-1832 (1999).	Isomerization C_2H_2 Energy Calculations
80625.	Miyoshi, A., N. Yamauchi, K. Kosaka, M. Koshi and H. Matsui, "Two-Channel Thermal Unimolecular Decomposition of Alkyl Iodides," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 46-53 (1999).	Unimolecular Dissociation RI R=C_2-C_4 Alkyl Channels Rate Constants Branching Ratios
80626.	Ben-Nun, M., and T.J. Martinez, "Ab Initio Molecular Dynamics Study of *cis-trans* Photoisomerization in Ethylene," *Chem. Phys. Lett.* 298, 57-65 (1998).	Photoisomerization *cis/trans* C_2H_4 Quenching Calculations
80627.	Derecskei-Kovacs, A., and S.W. North, "The Unimolecular Dissociation of Vinylcyanide: A Theoretical Investigation of a Complex Multichannel Reaction," *J. Chem. Phys.* 110, 2862-2871 (1999).	Unimolecular Dissociation C_2H_3CN P.E. Surfaces Channels Rates

80628. Zhong, D., E.W.-G. Diau, T.M. Bernhardt, S. De Feyter, J.D. Roberts and A.H. Zewail, "Femtosecond Dynamics of Valence-Bond Isomers of Azines: Transition States and Conical Intersections," *Chem. Phys. Lett.* 298, 129-140 (1998).

Isomerization
Ring Opening
Azines, $C_3H_3N_3$
$C_4H_4N_2$, C_5H_5N
fs Absorptions

(80778) Isomerization Energies, Fragmentations, Structural Calculations

$CH_3CNCH_2^+$/
$CH_3NCCH_2^+$

80629. McAdoo, D.J., S. Olivella and A. Sole, "Theoretical Analysis of the Unimolecular Gas Phase Decomposition of the Propane Molecular Ion," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10798-10804 (1998).

Unimolecular
Dissociation
$C_3H_8^+$
Rate Constants
Channels
Calculations

80630. Dubnikova, F., and A. Lifshitz, "Isomerization of Pyrrole: Quantum Chemical Calculations and Kinetic Modeling," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10880-10888 (1998).

Isomerization
c-C_4H_4NH
Channels
Rate Constants
RRKM Analysis

80631. Chesko, J.D., and Y.T. Lee, "Unimolecular Decay of Azabenzene: A Mechanistic Model Based on Pyrazine's Photoreactive Relaxation Pathways," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 107-120 (1997).

Unimolecular
Dissociation
c-$C_4H_4N_2$
Products
Energies
Mechanism

80632. Kalra, B.L., J.Y. Cho and D.K. Lewis, "Kinetics of the Thermal Isomerization of Methylcyclopropane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 362-364 (1999).

Unimolecular
Isomerization
c-$C_3H_5(CH_3)$
Channels
Rate Constants
Temperature
Dependences

80633. Mazyar, O.A., and T. Baer, "Isomerization and Dissociation in Competition: The Two-Component Dissociation Rates of Methyl Propionate Ions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1221-1227 (1999).

Unimolecular
Isomerization
$C_2H_5COOCH_3^+$
IP($C_2H_5COOCH_3$)
$\Delta H_f(C_2H_5CO^+)$
Channels

80634. Lendvay, G., and B. Viskolcz, "Ab Initio Studies of the Isomerization and Decomposition Reactions of the 1-Butoxy Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10777-10786 (1998).

Unimolecular
Isomerization
C_4H_9O
Rate Constants
Channels

80635. Urbain, P., B. Leyh, F. Remacle, A.J. Lorquet, R. Flammang and J.C. Lorquet, "Unimolecular Reaction Dynamics from Kinetic Energy Release Distributions. III. A Comparative Study of the Halogenobenzene Cations," *J. Chem. Phys.* 110, 2911-2921 (1999).

Unimolecular Dissociation
$C_6H_5X^+$
Product X Atom Kinetic Energies
X=Cl,Br,I

80636. Lifshitz, A., C. Tamburu and R. Shashua, "Thermal Decomposition of 2,5-Dimethylfuran: Experimental Results and Computer Modeling," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10655-10670 (1998).

Unimolecular Dissociation
c-$C_4H_2O(CH_3)_2$
Rate Constants
Products
Shock Tube
Kinetic Modeling

80637. Okuno, Y., "A Statistical Rate Constant Calculation Method Based on Monte Carlo Transition State Theory and Application to Unimolecular Dissociation of HFCO," *J. Chem. Phys.* 110, 2778-2784 (1999).

Unimolecular Dissociation
HFCO
Rate Constant Calculation Method

80638. Hauschildt, J., J. Weiss, C. Beck, S.Yu. Grebenshchikov, R. Duren, R. Schinke and J. Koput, "Unimolecular Dissociation of HOCl: Unexpectedly Broad Distribution of Rate Constants," *Chem. Phys. Lett.* 300, 569-576 (1999).

Unimolecular Dissociation
HOCl
P.E. Surface
Rate Constants Calculations

80639. Gutierrez-Oliva, S., J.R. Letelier and A. Toro-Labbe, "Energy, Chemical Potential and Hardness Profiles for the Rotational Isomerization of HOOH, HSOH and HSSH," *Mol. Phys.* 96, 61-70 (1999).

Isomerizations
H_2O_2, H_2S_2
HSOH
Energy Barriers
Mechanisms
Calculations

80640. Karan, K., A.K. Mehrotra and L.A. Behie, "On Reaction Kinetics for the Thermal Decomposition of Hydrogen Sulfide," *AIChE J.* 45, 383-389 (1999).

Unimolecular Dissociation
H_2S+M
Rate Constants
T Dependence
Quartz Reactor

80641. Arranz, F.J., F. Borondo and R.M. Benito, "Molecular Spectra, Quantum Chaos, and Scars," *Eur. Phys. J. D* 4, 181-187 (1998).

Isomerization
LiNC/LiCN
Regularity/ Chaos
Modeling

80642. Manz, J., K. Sundermann and R. de Vivie-Riedle, "Quantum Optimal Control Strategies for Photoisomerization via Electronically Excited States," *Chem. Phys. Lett.* 290, 415-422 (1998).

Photoisomerization
Li_2Na
Control Theory

80643. Chalk, A.J., and L. Radom, "Ion-Transport Catalysis: Catalyzed Isomerizations of NNH^+ and $NNCH_3^+$," *J. Am. Chem. Soc.* 121, 1574-1581 (1999).

Isomerization
NNH^+
$NNCH_3^+$
Neutral Molecule
Catalysis
Barrier Lowering
Mechanism

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

80644. Durant, J.L., "Computational Thermochemistry and Transition States," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 267-284 (1998).

Reaction Dynamics
Transition States
Frequencies
Energies
Calculations

80645. Chuang, Y.-Y., J.C. Corchado and D.G. Truhlar, "Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction Path Dynamics Methods," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1140-1149 (1999).

Reaction Dynamics
Path Approximations
Single Point
Calculation
Methods

80646. Frishman, E., M. Shapiro and P. Brumer, "Coherent Enhancement and Suppression of Reactive Scattering and Tunneling," *J. Chem. Phys.* 110, 9-11 (1999).

Reaction Dynamics
Coherent Control
Theory

80647. Petersson, G.A., "Complete Basis-Set Thermochemistry and Kinetics," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 237-266 (1998).

Reaction Dynamics
Transition State
Energies
$D,F,OH + H_2$
$H + D_2, H_2O$
Activation Energy
Calculations

80648. Stockigt, D., "The Mechanism of the Gas Phase Ion-Molecule Reaction Between Al^+ and Ethanol," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10493-10500 (1998).

Reaction Dynamics
$Al^+ + C_2H_5OH$
Channels
Energies

80649. Bell, R., and J. Simons, "Unusual Thresholds and Isotope Effects in $Al^+ + H_2/D_2/HD$ Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 539-549 (1999).

Reaction Dynamics
$Al^+ + H_2, HD, D_2$
P.E. Surface
Mechanism

80650. Lesar, A, and M. Hodoscek, "Ab Initio Molecular Orbital and Density Functional Characterization of the Potential Energy Surface of the $N_2O + Br$ Reaction," *J. Chem. Phys.* 109, 9410-9416 (1998).

Reaction Dynamics
$Br + N_2O$
P.E. Surface
Activation Energy

80651. Chistyakov, A.L., I.V. Stankevich, N.P. Gambaryan and I.S. Akhrem, "MNDO/PM3 Study of the Mechanism of a Model Reaction between Methane and Br^+ Cation," *Russ. Chem. Bull.* 47, 1666-1669 (1998).

Reaction Dynamics
$Br^+ + CH_4$
P.E. Surface
Energies
Channels

80652. Polak, R., "The Diatomics-in-Molecules Method as a Means for Predicting Potential Energy Surface Topology: A Case Study for the Reaction of C^+ with O_2," *Collect. Czech. Chem. Commun.* 63, 1329-1342 (1998).

Reaction Dynamics
$C^+ + O_2$
P.E. Surface
Energies

80653. Moon, J.H., S.T. Park and M.S. Kim, "Classical Trajectory Study of $CD_2OH^+ \rightarrow CDO^+ + HD$ on Potential Energy Surfaces Constructed at Various Quantum Chemical Levels: Scaling of Product Mode-Specific Energies," *J. Chem. Phys.* 110, 972-977 (1999).

Reaction Dynamics
CD_2OH^+
Dissociation
P.E. Surfaces
Energy Barriers

80654. Wang, Z.-X., and M.-B. Huang, "A G2 Study on CH Insertions into PH_3, H_2S and HCl," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 265-271 (1999).

Reaction Dynamics
$CH + HCl, HF$
$CH + H_2O, H_2S$
$CH + NH_3, PH_3$
Insertion Energies
Mechanisms

80655. Chakraborty, D., and M.C. Lin, "Theoretical Studies of Methyleneamino (CH_2N) Radical Reactions. I. Rate Constants and Product Branching Ratios for the $CH_2N + N_2O$ Process by ab Initio Molecular Orbital/Statistical Theory Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 601-606 (1999).

Reaction Dynamics
$CH_2N + N_2O$
Channels
Rate Constant
Calculations

80656. Minyaev, R.M., A.G. Starikov and E.A. Lepin, "Pathways of the Reactions of Nucleophilic Addition of H_2O and HF Molecules to Formaldehyde in the Gas Phase and in the Complex with Formic Acid: Ab Initio Calculations," *Russ. Chem. Bull.* 47, 2078-2086 (1998).

Reaction Dynamics
$CH_2O + HF$
$CH_2O + H_2O$
Pathways
Activation
Energies

80657. Yamataka, H., M. Aida and M. Dupuis, "One Transition State Leading to Two Product States: Ab Initio Molecular Dynamics Simulations of the Reaction of Formaldehyde Radical Anion and Methyl Chloride," *Chem. Phys. Lett.* 300, 583-587 (1999).

Reaction Dynamics
$CH_2O^- + CH_3Cl$
Transition State
Branching Channels
2 Product States

80658. Arnaud, R., V. Vetere and V. Barone, "Regioselectivity of Methyl Radical Addition to Fluoroethenes: A Quantum Mechanical Study," *Chem. Phys. Lett.* 293, 295-301 (1998).

Reaction Dynamics
$CH_3 + C_nH_{2n-m}F_m$
$m = 1\text{-}3$
Regioselectivity
Energies

80659. Espinosa-Garcia, J., E.L. Coitino, A. Gonzalez-Lafont and J.M. Lluch, "Reaction Path and Dual-Level Dynamics Calculations of the CH_3F+OH Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10715-10722 (1998).

Reaction Dynamics
CH_3F+OH
Rate Constants
Reaction Path
$H_2O(v)$ Product
Calculations

80660. Bofill, J.M., S. Olivella, A. Sole and J.M. Anglada, "The Mechanism of Methoxy Radical Oxidation by O_2 in the Gas Phase: Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent O···O Bonding Interaction," *J. Am. Chem. Soc.* 121, 1337-1347 (1999).

Reaction Dynamics
CH_3O+O_2
Rate Constants
P.E. Surface
Channels

80661. Schiesser, C.H., and M.A. Skidmore, "On the Mechanism of 'Polarity Reversal Catalysis': An ab Initio Study of Hydrogen Atom Transfer Between Silane and Methylthiyl Radicals," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 2329-2331 (1998).

Reaction Dynamics
CH_3S+SiH_4
Energy Barrier

80662. Harding, L.B., and S.J. Klippenstein, "A Theoretical Analysis of the Reaction of H with C_2H_5," *Int. Symp. Combust.* 27, 151-157 (1998).

Reaction Dynamics
C_2H_5+H
Channels
Rate Constant
Calculations

80663. Yamada, T., J.W. Bozzelli and T. Lay, "Thermodynamic and Kinetic Analysis Using ab Initio Calculations on Dimethyl Ether Radical$+O_2$ Reaction System," *Int. Symp. Combust.* 27, 201-209 (1998).

Reaction Dynamics
$CH_3OCH_2+O_2$
Rate Constants
Channels
$\Delta H_f(CH_3OCH_2)$
$\Delta H_f(CH_3OCH_2O_2)$
$\Delta H_f(CH_2OCH_2OOH)$
Calculations

80664. Sobolewski, A.L., and W. Domcke, "On the Mechanism of Rapid Non-Radiative Decay in Intramolecularly Hydrogen-Bonded π Systems," *Chem. Phys. Lett.* 300, 533-539 (1999).

Reaction Dynamics
$CH_2(CHO)_2$
Singlet State
H-Atom Transfer
P.E. Surfaces
Efficient Relaxation
Channel

80665. Hertwig, R.H., and W. Koch, "A Theoretician's View of the C-F Bond Activation Mediated by the Lanthanide Cations Ce^+ and Ho^+," *Chem. Eur. J.* 5, 312-319 (1999).

Reaction Dynamics
$Ce^+ + CH_3F, C_6H_5F$
$Ho^+ + CH_3F, C_6H_5F$
Paths
Energies

80666. Chen, M.-D., M.-L. Wang, K.-L. Han and S.-L. Ding, "Theoretical Studies of Scattering-Angle Resolved Product Rotational Alignment for the Reaction of Cl with Vibrationally Excited Methane," *Chem. Phys. Lett.* 301, 303-308 (1999).

Reaction Dynamics
$Cl+CH_4(v)$
Product HCl(J)
Alignment
Calculations

80667. Hwang, D.-Y., and A.M. Mebel, "Ab Initio Study on the Reaction Mechanism of Ozone with the Chlorine Atom," *J. Chem. Phys.* 109, 10847-10852 (1998).

Reaction Dynamics
$Cl + O_3$
P.E. Surface
Rate Constants
Energy Barrier

80668. Manuel, M., O. Mo and M. Yanez, "The Reactions of $Cl^+(^3P)$ and $Cl^+(^1D)$ with Hydrogen Sulfide: A G2 Molecular Orbital Study," *Mol. Phys.* 96, 231-241 (1999).

Reaction Dynamics
$Cl^+(^1D,^3P) + H_2S$
P.E. Surfaces
Energies
$\Delta H_f(H_2SCl^+)$

80669. Thompson, W.H., "Direct Calculation of Reactive Thermal Rate Constants," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 304-318 (1997).

Reaction Dynamics
$D + H_2$
Rate Constant
Direct
Calculation Method

80670. Meijer, A.J.H.M., E.M. Goldfield, S.K. Gray and G.G. Balint-Kurti, "Flux Analysis for Calculating Reaction Probabilities with Real Wave Packets," *Chem. Phys. Lett.* 293, 270-276 (1998).

Reaction Dynamics
$D + H_2$
3-D Scattering
Probabilities
Method

80671. Adhikari, S., and G.D. Billing, "The Geometric Phase Effect on Differential Cross Sections in Chemical Reactions: A Classical Mechanical Approach," *Chem. Phys. Lett.* 289, 219-223 (1998).

Reaction Dynamics
$D + H_2$
Conical
Intersection
Geometric Phase
Effects

80672. Kornweitz, H., A. Persky and R.D. Levine, "The Exoergic $F + CH_4$ Reaction as an Example of Peripheral Dynamics," *Chem. Phys. Lett.* 289, 125-132 (1998).

Reaction Dynamics
$F + CH_4$
$F + H_2$
HF(v) Product
Forward Scattering
Trajectories

80673. Rutenburg, I., and G.W. Koeppl, "Application of a General Classical Variational Theory to the $F + H_2 \rightarrow FH + H$ Reaction," *J. Chem. Phys.* 110, 3842-3855 (1999).

Reaction Dynamics
$F + H_2$
General Theory
Accuracies

80674. Pais, A.A.C.C., L.G. Arnaut and S.J. Formosinho, "Hydrogen-Atom Abstractions: A Semiempirical Approach to Reaction Energetics, Bond Lengths and Bond Orders," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 2577-2584 (1998).

Reaction Energetics
H-Atom Transfer
Activation Energies
Estimation
Method

80675. Aoiz, F.J., B. Friedrich, V.J. Herrero, V.S. Rabanos and J.E. Verdasco, "Effect of Pendular Orientation on the Reactivity of H+DCl: A Quasiclassical Trajectory Study," *Chem. Phys. Lett.* 289, 132-140 (1998).

Reaction Dynamics
H+DCl
Channels
Competing
Mechanisms

80676. Jackle, A., M.-C. Heitz and H.-D. Meyer, "Reaction Cross Sections for the $H+D_2(v=0,1)$ System for Collision Energies up to 2.5 eV: A Multiconfiguration Time-Dependent Hartree Wavepacket Propagation Study," *J. Chem. Phys.* 110, 241-248 (1999).

Reaction Dynamics
$H+D_2(v,J)$
Cross Sections
Reactant Energy
Effects

80677. Varandas, A.J.C., and P.E. Abreu, "Quasi-ab Initio Dynamics: A Test Trajectory Study of the $H+H_2$ Reaction Using Energies and Gradients Based on Scaling of the External Correlation," *Chem. Phys. Lett.* 293, 261-269 (1998).

Reaction Dynamics
$H+H_2$
Exchange Reaction
Calculation Method

80678. Lendvay, G., K.S. Bradley and G.C. Schatz, "Reactive and Inelastic Collisions of H Atoms with Vibrationally Excited Water Molecules," *J. Chem. Phys.* 110, 2963-2970 (1999).

Reaction Dynamics
$H+H_2O(v)$
Vibrational
Effects
Rate Constants
Reactive/
Inelastic Channels

80679. Meijer, A.J.H.M., and E.M. Goldfield, "Time-Dependent Quantum Mechanical Calculations on $H+O_2$ for Total Angular Momentum $J>0$. II. On the Importance of Coriolis Coupling," *J. Chem. Phys.* 110, 870-880 (1999).

Reaction Dynamics
$H+O_2(J)$
Cross Sections
J Effects

80680. Ansari, W.H., and N. Sathyamurthy, "Classical Mechanical Investigation of Colinear $H^-+H_2 \rightarrow H_2+H^-$ Dynamics," *Chem. Phys. Lett.* 289, 487-493 (1998).

Reaction Dynamics
H^-+H_2,D_2
Probabilities
Collision Energy
Dependences

80681. Bruno, D., M. Capitelli and S. Longo, "Direct Simulation Monte Carlo Modeling of Vibrational and Chemical Kinetics for a Reacting Gas Mixture," *Chem. Phys. Lett.* 289, 141-149 (1998).

Reaction Dynamics
H_2+Xe
Vibrational
Nonequilibrium
Simulation
Method

80682. Kumar, S., H. Kapoor and N. Sathyamurthy, "Dynamics of the Reaction $He+H_2^+ \rightarrow HeH^++H$ on the Aguado-Paniagua Surface," *Chem. Phys. Lett.* 289, 361-366 (1998).

Reaction Dynamics
$H_2^+(v)+He$
Probabilities
Collisional Energy
Dependences

80683. Krokidis, X., B. Silvi, C. Dezarnaud-Dandine and A. Sevin, "Topological Study, Using a Coupled Electron Localization Function and Catastrophe Theory Technique, of Electron Transfer in the $Li+Cl_2$ System," *New J. Chem.* 1341-1350 (1998).

Reaction Dynamics
$Li+Cl_2$
Electron Transfer
Harpooning Process

80684. Lara, M., A. Aguado, O. Roncero and M. Paniagua, "Quantum Stereodynamics of the Li+HF(v,j) Reactive Collision for Different Initial States of the Reagent," *J. Chem. Phys.* 109, 9391-9400 (1998).

Reaction Dynamics
Li+HF(v,J)
Cross Sections
Energy Effects

80685. Topaler, M.S., T.C. Allison, D.W. Schwenke and D.G. Truhlar, "Erratum - What is the Best Semiclassical Method for Photochemical Dynamics of Systems with Conical Intersections? [*J. Chem. Phys.* 109, 3321-3345 (1998)]," *ibid.* 110, 687-688 (1999).

Reaction Dynamics
$M^*+H_2/M+H_2(v,J)$
$M^*+H_2/MH+H$
Conical Intersections
Erratum

80686. Kurosaki, Y., and T. Takayanagi, "Ab Initio Molecular Orbital Study of the $N(^2D)+H_2O$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 436-442 (1999).

Reaction Dynamics
$N(^2D)+H_2O$
Channels
Energies

80687. Russell, C.L., and D.E. Manolopoulos, "Time-Dependent Wavepacket Study of the N^++H_2 Reaction," *J. Chem. Phys.* 110, 177-187 (1999).

Reaction Dynamics
$N^++H_2(v=0,1)$
Rate Constants
P.E. Surface
Calculations

80688. Zhang, Y.C., L.X. Zhan, Q.G. Zhang, W. Zhu and J.Z.H. Zhang, "Quantum Wavepacket Calculation for the Ion Molecule Reaction $N^++H_2=NH^++H$," *Chem. Phys. Lett.* 300, 27-32 (1999).

Reaction Dynamics
$N^++H_2(J)$
P.E. Surface
Probabilities

80689. Szichman, H., M. Baer, H.R. Volpp and J. Wolfrum, "Comparison Between Experimental and Three-Dimensional Quantum Mechanical Rate Constants for the NH(D)+NO Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10455-10459 (1998).

Reaction Dynamics
NH+NO
ND+NO
Rate Constants
T Dependences
Calculations

80690. Szichman, H., M. Baer, H.-R. Volpp and J. Wolfrum, "Three-Dimensional Quantum Mechanical Study of the $NH(X^3\Sigma^-)+NO$ Reaction," *Int. Symp. Combust.* 27, 253-259 (1998).

Reaction Dynamics
NH+NO
Rate Constants
Branching
Calculations

80691. Tachibana, A., and M. Fuju, "A Simple Algorithm for Conservation of Invariants of Motion in Reaction Dynamics Calculations: Application to the $NH_3^++NH_3$ System," *J. Chem. Phys.* 110, 2323-2331 (1999).

Reaction Dynamics
$NH_3^++NH_3$
Energy Conservation
Algorithm
Angular Momentum
Role

80692. Manaa, M.R., C.F. Chabalowski, "A Theoretical Treatment of the Intersystem Crossing in the Spin Forbidden Reaction $NO(X^2\Pi)+CO(X^1\Sigma^+)\rightarrow N(^4S)+CO_2(X^1\Sigma_g^+)$," *Chem. Phys. Lett.* 300, 619-625 (1999).

Reaction Dynamics
NO+CO
N Product Channel
Energetics
Curve Crossings

80693. Mil'nikov, G.V., C. Zhu, H. Nakamura and V.I. Osherov, "Semiclassical Treatment of Resonances in the Colinear O+HO Exchange Reaction," *Chem. Phys. Lett.* 293, 448-454 (1998).

Reaction Dynamics
O+OH
Resonances
Curve Crossing
Calculations

80694. Gonzalez, M., D. Troya, M.P. Puyuelo, R. Sayos and P.A. Enriquez, "The Dynamics of the $O(^1D)+N_2O\rightarrow NO+NO$ Reaction Revisited: A QCT Study on Model Potential Energy Surfaces," *Chem. Phys. Lett.* 300, 603-612 (1999).

Reaction Dynamics
$O(^1D)+N_2O$
Cross Sections
NO(v) Product
Distributions

80695. Masgrau, L., A. Gonzalez-Lafont and J.M. Lluch, "Mechanism of the Gas Phase $HO+H_2O\rightarrow H_2O+OH$ Reaction and Several Associated Isotope Exchange Reactions: A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1044-1053 (1999).

Reaction Dynamics
$OH+H_2O$
Exchange
Isotopic Effects
Rate Constants

80696. Campos-Martinez, J., E. Carmona-Novillo, J. Echave, M.I. Hernandez, R. Hernandez-Lamoneda and J. Palma, "Reaction and Inelastic Processes in the Collision $O_2(v\gg0)+O_2(v=0)$," *Eur. Phys. J. D* 4, 159-168 (1998).

Reaction Dynamics
$O_2(v\gg0)+O_2$
Channels
Rate Constants
Vibrational
Relaxation
Dominance

80697. Horie, O., and G.K. Moortgat, "Gas Phase Ozonolysis of Alkenes: Recent Advances in Mechanistic Investigations," *Acc. Chem. Res.* 31, 387-396 (1998).

Reaction Dynamics
O_3+Alkenes
Mechanism
Review

80698. Lendvay, G., and I. Mayer, "Some Difficulties in Computing BSSE-Corrected Potential Surfaces of Chemical Reactions," *Chem. Phys. Lett.* 297, 365-373 (1998).

Reaction Dynamics
PH_3+H
Barrier Heights
P.E. Surface
Difficulties

80699. Lu, W.C., C.B. Liu and C.C. Sun, "Theoretical Study of the H_3PNH+H_2CO Reaction Mechanism via Five Reaction Channels," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1078-1083 (1999).

Reaction Dynamics
$PH_3(NH)+HCHO$
Channels
Energies

80700. Kalus, R., "Collisions of Noble Gas Dimers with Monomers: A Classical Trajectory Study," *J. Chem. Phys.* 110, 3856-3860 (1999).

Reaction Dynamics
Rg_2+Rg
Rate Constants
Calculations

80701. Stirling, A., "Theoretical Calculations on the Reactions of NO_2 with Sc, Ti and V," *Chem. Phys. Lett.* 298, 101-106 (1998).

Reaction Dynamics
Sc,Ti + NO_2
V + NO_2
Mechanisms

80702. Irigoras, A., J.E. Fowler and J.M. Ugalde, "Reactivity of $Sc^+(^3D,^1D)$ and $V^+(^5D,^3F)$: Reaction of Sc^+ and V^+ with Water," *J. Am. Chem. Soc.* 121, 574-580 (1999).

Reaction Dynamics
$Sc^+,V^+ + H_2O$
$Sc^+(^1D),V^+(^3F) + H_2O$
Spin Effects
Channels

80703. Salazar, M.R., and J. Simons, "Reactive Dynamics for $Zn(^3P) + H_2/D_2/HD \rightarrow ZnH/ZnD + H/D$: Rotational Populations in ZnH/ZnD Products," *J. Chem. Phys.* 110, 229-240 (1999).

Reaction Dynamics
$Zn^*(^3P) + H_2,HD,D_2$
ZnH,ZnD(v,J)
Product Distributions
Calculations
Data Comparisons

41. CHEMICAL KINETICS - GENERAL

(See also Section 42 for Reaction Control Methods)

80704. Till, U., C.R. Timmel, B. Brocklehurst and P.J. Hore, "The Influence of Very Small Magnetic Fields on Radical Recombination Reactions in the Limit of Slow Recombination," *Chem. Phys. Lett.* 298, 7-14 (1998).

$^1A + ^1B$
Singlet Radical
Recombinations
Magnetic Field
Effects

(80435) Absorption Measurements, $Ar^*(1s_5)$ Decay Rates

Ar Plasma

80705. Sasaki, K., K. Usui, H. Furukawa, C. Suzuki and K. Kadota, "Lifetime Measurements of CF_x Radicals and H Atoms in Afterglow of CF_4/H_2 Plasmas," *Jpn. J. Appl. Phys.* 37, 5047-5048 (1998).

CF,CF_2,H
Radical Decay
Time Constants
CF_4/H_2 Discharge
Kinetics

(80492) C_4F_8 Discharge, Measurements

CF,CF_2, LIF
F, VUV Absorption

(80839) $\Delta H_{Reaction}$, Calculations, $\Delta H_f(CH_nX_{4-n},CH_nF_mCl_p,C_2H_nF_{6-n},C_2H_nF_{4-n})$

Halocarbons + H,OH

80706. Koffi-Kpante, K., D. Zeitoun and L. Labracherie, "Computation and Experimental Validation of N_2/CH_4/Ar Mixture Flows Behind Normal Shock Wave," *Shock Waves* 7, 351-361 (1997).

CH_4/N_2/Ar
Shock Heated
Nonequilibrium
Dissociation/
Vibration
Flow Modeling

80707. Garland, N.L., and S.W. McElvany, "Ionization Potentials of TNAZ (1,3,3-Trinitroazetidine) and Its Decomposition Products," *Chem. Phys. Lett.* 297, 147-153 (1998).

$C_3H_4N(NO_2)_3$
Thermal Dissociation
Products
IPS(Parent/Products)

80708.	McDowell, D.R., F. Wu and R.B. Weisman, "A New Method for Measuring Vibrational Energy Distributions of Polyatomics," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 191-201 (1997).	*c*-$C_4H_4N_2$ Vibrational Energy Distributions Polyatomics Decay Rate Interpretation New Method
80709.	Goldaniga, A., T. Faravelli, E. Ranzi, P. Dagaut and M. Cathonnet, "Methyl and Ethyl Tertiary Butyl Ethers, Di-isopropyl Ether and Tertiary Amyl Methyl Ether," *Int. Symp. Combust.* 27, 353-360 (1998).	(i-C_3H_7)$_2$O *t*-$C_4H_9OCH_3$ *t*-$C_4H_9OC_2H_5$ *t*-$C_5H_{11}OCH_3$ Oxidation Kinetics Stirred Reactor Products Mechanisms
(80879)	Movable Nozzle, Microwave Method	H-Atom Source
80710.	Loura, B.B., and F. Olga, "Thermal Oxidation of Hydrogen Sulfide," *J. de Chim. Phys.* 95, 1991-2000 (1998).	H_2S/O_2 ,SO_2 Thermal Oxidation Rates 620-970 K SO_2 Formation
(80339)	Zeldovich Mechanism, Hypersonic Flows, Nonequilibrium Effects	NO Formation
(80338)	Nonequilibrium Relaxation Effects, Supersonic Air, Nozzle Flow	NO Formation
80711.	Hori, M., N. Matsunaga, N. Marinov, W. Pitz and C. Westbrook, "An Experimental and Kinetic Calculation of the Promotion Effect of Hydrocarbons on the NO-NO_2 Conversion in a Flow Reactor," *Int. Symp. Combust.* 27, 389-396 (1998).	NO/NO_2 Conversion C_1-C_3 Hydrocarbon Oxidation Kinetics Role
(80451)	Kinetic Model, $N_2(B,v)+N_2$ Quenching Rate Constants	N_2 Discharge
(80643)	NNH^+, $NNCH_3^+$ Isomerizations, Induced Energy Barrier Lowering Mechanism	Neutral Molecule Catalysis
80712.	Politzer, P., and J.M. Seminario, "Use of Density Functional Methods to Compute Heats of Reactions," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 359-368 (1998).	$NH_4N(NO_2)_2$,(c) Dissociation $\Delta H_{Reaction}$,Channels Calculations
80713.	Fajgar, R., J. Vitek, Y. Haas and J. Pola, "Formation of Secondary Ozonides in the Gas Phase Low Temperature Ozonation of Primary and Secondary Alkenes," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 239-248 (1999).	O_3+RH Alkenes Product Secondary Ozonides FTIR Yields

80714. Das, U.K., and P. Chaudhuri, "Optical Emission Spectroscopic Study of a Radiofrequency Plasma of $Ar+SiH_4$," *Chem. Phys. Lett.* 298, 211-216 (1998).

SiH_4/Ar
RF Discharge
Product
Ar*,SiH(A-X)
Modeling

42. LASERS/INDUCED EFFECTS/MPI

80715. Sibbett, W., D.T. Reid and M. Ebrahimzadeh, "Versatile Femtosecond Laser Sources for Time-Resolved Studies: Configurations and Characterizations," *Phil. Trans. Roy. Soc. Lond. A* 356, 283-296 (1998).

fs Laser Sources
Tunable
Review

80716. Zhou, J.X., X. Hou, K.X. Yang, S.-J.J. Tsai and R.G. Michel, "Lasers Based on Optical Parametric Devices: Wavelength Tunability Empowers Laser Based Techniques in the Ultraviolet, Visible and Near-Infrared," *Appl. Spectrosc.* 52, 176A-189A (1998).

OPD
Tunable Laser Sources
Review

80717. Wolfrum, J., "Lasers in Combustion: From Basic Theory to Practical Devices," *Int. Symp. Combust.* 27, 1-41 (1998).

Laser Diagnostic Techniques
Combustion Applications
Review

(80646) Reaction Dynamics, Theory

Coherent Control

80718. Stolow, A., "Applications of Wavepacket Methodology," *Phil. Trans. Roy. Soc. Lond. A* 356, 345-362 (1998).

Wavepacket Techniques
Applications
Review

80719. Riffe, D.M., and A.J. Sabbah, "A Compact Rotating Mirror Autocorrelator Design for Femtosecond and Picosecond Laser Pulses," *Rev. Sci. Instrum.* 69, 3099-3102 (1998).

fs,ps Laser Pulse
Rotating Mirrors
Interferometric Autocorrelator
Compact Design

(80574) Resonant/Nonresonant Differences, Calculations

2-Photon (Color) Dissociation

80720. Liu, L., and J.T. Muckerman, "Strong-Field Optical Control of Vibrational Dynamics: Vibrational Stark Effect in Planar Acetylene," *J. Chem. Phys.* 110, 2446-2451 (1999).

IR Laser Control
$C_2H_2(\nu_{CH})$ Pump
Formation of $3\nu_{C-C}$ Stretch
Polarized 2-Pulse Scheme

80721. Assion, A., T. Baumert, M. Geisler, V. Seyfried and G. Gerber, "Mapping of Vibrational Wavepacket Motion by Femtosecond Time Resolved Kinetic Energy Time-of-Flight Mass Spectroscopy," *Eur. Phys. J. D* 4, 145-149 (1998).

fs Pump/Probe
TOF Mass Analysis
$Na_2(2^1\Sigma_u^+)$
Vibrational Wavepacket Dynamics

(80376) Nomenclature Recommendations, Laser Atomic Spectroscopy — MPI,LIF

(80471) (2+1) Mode, Monitor Sensitivity — REMPI,CO

(80820) Free Jets, CO/CO,He,Ar,N_2, Rotational Relaxation, CO(J) Distributions — REMPI,CO(J)

(80584) fs MPD/MPI, Product Ions, Fragmentations, Measurements — *c*-C_3H_6,C_6H_6 *c*-C_6H_{12}

(80440) C_4H_2*+C_2H_4,C_3H_6,C_4H_2 Reaction Products, Product Ionization Thresholds — R2PI Spectra C_6H_2,C_6H_4 C_7H_6,C_8H_2

(80472) REMPI/TOFMS, Incinerator On-line Flue Gas Monitor — $C_{10}H_8$,PAHs

(80421) Rydberg State Spectra, Measurements — REMPI/PES,NH_3

(80614) N_2(v=0,J=40-90), N_2(v=1) Photofragment Anisotropies, N_2O+hν, Measurements — REMPI,N_2

(80594) Pathway Control, fs Pump/Probe, NaK^+, Na^+ Channels, P.E. Curves — MPI,NaK

(80615) (3+1),(2+1) Ion Imaging, O_3+hν(276 nm), Product Distributions, Alignments — REMPI,O(^{1}D)

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects, Section 40 for Surface Dynamics)

80722. Chang, E.S., and M. Geller, "Improved Experimental Energy Levels of Carbon(I) from Solar Infrared Spectra," *Phys. Scr.* 58, 326-340 (1998).
Energy Levels
C
356 Lines
IR Spectral Analysis

80723. Gordillo-Vazquez, F.J., and J.A. Kunc, "High-Accuracy Expressions for Rotational-Vibrational Energies of O_2, N_2, NO and CO Molecules," *J. Thermophys. Heat Transfer* 12, 52-56 (1998).
v,J Energy Levels
CO,NO
N_2,O_2
Accurate Expressions

80724. Zuniga, J., A. Bastida, M. Alacid and A. Requena, "Optimal Generalized Internal Vibrational Coordinates for Symmetrical Linear Triatomic Molecules," *Chem. Phys. Lett.* 298, 36-42 (1998).
Vibrational Energy Levels
CO_2,CS_2
Calculations

80725. Peric, M., and J. Radic-Peric, "Ab Initio Investigation of the Vibronic Structure and the Spin-Orbit Coupling in the $X^2\Pi_u$ State of $C_2D_2^+$," *Chem. Phys. Lett.* 290, 443-450 (1998).
Vibrational Energy Levels
$C_2D_2^+$(X)
Renner-Teller Effect

80726. El Idrissi, M.I., J. Lievin, A. Campargue and M. Herman, "The Vibrational Energy Pattern in Acetylene. IV. Updated Global Vibration Constants for $^{12}C_2H_2$," *J. Chem. Phys.* 110, 2074-2086 (1999).

Vibrational Energy Levels
$C_2H_2(X)$
Data Set
Model Fitting

80727. Jacobson, M.P., R.J. Silbey and R.W. Field, "Local Mode Behavior in the Acetylene Bending System," *J. Chem. Phys.* 110, 845-859 (1999).

$C_2H_2(X)$
Bending Mode
Description
$\leq$15000 cm^{-1}

80728. Skokov, S., J. Qi, J.M. Bowman, C.-Y. Yang, S.K. Gray, K.A. Peterson and V.A. Mandelshtam, "Accurate Variational Calculations and Analysis of the HOCl Vibrational Energy Spectrum," *J. Chem. Phys.* 109, 10273-10283 (1998).

Vibrational Energy Levels
HOCl
IR Intensities
Calculations

80729. Csaszar, A.G., J.S. Kain, O.L. Polyansky, N.F. Zobov and J. Tennyson, "Relativistic Correction to the Potential Energy Surface and Vibration-Rotation Levels of Water," *Chem. Phys. Lett.* 293, 317-323 (1998).

v,J Levels
H_2O
P.E. Surface
Calculations

80730. Mussa, H.Y., and J. Tennyson, "Calculation of the Rotation-Vibration States of Water up to Dissociation," *J. Chem. Phys.* 109, 10885-10892 (1998).

v,J Energy Levels
H_2O
Calculations

80731. Salzgeber, R.F., V.A. Mandelshtam, C. Schlier and H.S. Taylor, "All the Nonadiabatic (J=0) Bound States of NO_2," *J. Chem. Phys.* 110, 3756-3764 (1999).

Vibrational Energy Levels
NO_2(A,X)
Calculations

80732. Nakamura, H., and S. Kato, "Quantum Calculation of the Vibrational Energy Level Structure of N_2O Based on ab Initio Potential Surface," *Chem. Phys. Lett.* 297, 187-192 (1998).

Vibrational Energy Levels
N_2O
1647 Bound States
Calculations

(80793) v,J Energy Levels, P.E. Surface, Structural Calculations, Frequencies

$Si(H_2)O$

80733. Piela, L., "Search for the Most Stable Structures on Potential Energy Surfaces," *Collect. Czech. Chem. Commun.* 63, 1368-1380 (1998).

P.E. Surfaces
Energy Minima
Stable Structures
Algorithm

80734. Yarkony, D.R., "Conical Intersections: Diabolical and Often Misunderstood," *Acc. Chem. Res.* 31, 511-518 (1998).

P.E. Surfaces
Conical Intersections
$Al + H_2$
Review

80735. Chambaud, G., "Potential Energy Surfaces and Spectroscopy," *J. de Chim. Phys.* 95, 1892-1924 (1998).

P.E. Functions
Calculation Methods
$AlO,AlO^{\pm}$
HOCl,HOBr
HN_3,NO.Ar
Review

80736. Fernandez, B., and H. Koch, "Accurate ab Initio Rovibronic Spectrum of the $X^1\Sigma_g^+$ and $B^1\Sigma_u^+$ States in Ar_2," *J. Chem. Phys.* 109, 10255-10262 (1998).

P.E. Curves
Ar_2(B,X)
Spectral Constants
Energy Levels
D_0',D_0''

80737. Begue, D., M. Merawa, M. Rerat and C. Pouchan, "Long-Range Coefficients for the Low-lying Electronic States of BeLi and Be_2," *J. Chem. Phys.* 110, 2051-2058 (1999).

P.E. Curves
BeLi,Be_2
Low-lying States
Long Range Calculations

80738. Szalay, P.G., and L. Nemes, "Tunneling Lifetimes of the Rovibronic Levels in the B-Electronic State of the CH Radical Obtained from ab Initio Data," *Mol. Phys.* 96, 359-366 (1999).

P.E. Curves
CH(B,X)
Spectral Constants
B(v,N) State
Tunneling Lifetimes

80739. Sumathi, R., S.D. Peyerimhoff and D. Sengupta, "Rearrangement and Fragmentation Processes on the Potential Energy Surfaces of the CH_nS^+ (n=1-4) Systems," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 772-778 (1999).

P.E. Surfaces
CHS^+,CH_2S^+
CH_3S^+,CH_4S^+
Isomers
Stabilities
Stationary Points

(80623) P.E. Surface, Unimolecular Dissociation, Channels, Energies

CH_3OF

(80240) P.E. Curves, Dissociative Recombination Rate Constants, Branching Ratios

$CN^+(a,X)/e^-$

80740. Grein, F., "Ultraviolet and Photoelectron Spectrum of Carbonyl Fluoride, F_2CO: Multireference Configuration Interaction Studies in C_{2v} Symmetry," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10869-10879 (1998).

P.E. Curves
COF_2
Low-lying States
UV,PES Spectral Assignments
IP
COF_2^+ Frequencies

(80627) P.E. Surfaces, Unimolecular Dissociation, Channels, Rates

C_2H_3CN

(80799) P.E. Surfaces, Energy Relaxation, Mode Coupling, Calculations

c-$C_4H_4N_2(S_2)$

80741. Polly, R., D. Gruber, L. Windholz, M.M. Gleichmann and B.A. Hess, "Relativistic All-Electron ab Initio Calculations of CsHg Potential Energy Curves Including Spin-Orbit Effects," *J. Chem. Phys.* 109, 9463-9472 (1998).

P.E. Curves
CsHg
Low-lying States
Spectral Constants
D_e,Energies

80742. Li, Y., and J.S. Francisco, "A CASSCF-MRCI Study of the Electronically Excited States of FClO and FOCl," *J. Chem. Phys.* 110, 2404-2409 (1999).

P.E. Curves
FClO,FOCl
Low-lying States
Energies

80743. Shim, I., M.S. Baba and K.A. Gingerich, "Electronic Structure and Thermodynamic Properties of the Molecule GeC from All-Electron ab Initio Calculations and Knudsen Effusion Mass Spectrometric Measurements," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10763-10767 (1998).

P.E. Curves
GeC
Low-lying States
Spectral Constants
D_0,ΔH_f
Calculations

(80638) P.E. Surface, Unimolecular Dissociation, Rate Constants, Calculations

HOCl

80744. Nachtigallova, D., P. Slavicek, P. Nachtigall and P. Jungwirth, "Water Photolysis in Rare Gas Environment: the CASPT2 Excited State $H_2O(A)$-Ar Potential," *Collect. Czech. Chem. Commun.* 63, 1321-1328 (1998).

P.E. Surface
$H_2O(A).Ar_n$
Photodissociation
Dynamics

80745. Meuwly, M., and J.M. Hutson, "The Potential Energy Surface and Near-Dissociation States of He-H_2^+," *J. Chem. Phys.* 110, 3418-3427 (1999).

P.E. Surface
HeH_2^+
Calculations

(80800) P.E. Surfaces, Crossings, E-E Transfer, Calculations

$I(^2P_{1/2})+O_2$
$O_2(a)+I$

80746. Zanni, M.T., V.S. Batista, B.J. Greenblatt, W.H. Miller and D.M. Neumark, "Femtosecond Photoelectron Spectroscopy of the I_2^- Anion: Characterization of the $A'^2\Pi_{g,1/2}$ Excited State," *J. Chem. Phys.* 110, 3748-3755 (1999).

P.E. Curve
$I_2^-(A')$
fs Pump/Probe
PES
D_e,r_e

80747. Hoffman, G.J., L.A. Swafford and R.J. Cave, "An ab Initio Study of the Mono- and Difluorides of Krypton," *J. Chem. Phys.* 109, 10701-10706 (1998).

P.E. Curves
KrF,KrF^+
$^{1,3}KrF_2$,$Kr.F_2$
D_e,r_e

80748. Leung, A.W.K., R.R. Julian and W.H. Breckenridge, "The Lowest Energy $^3\Pi_{2,1,0^+,0^-}$ and $^3\Sigma_{1,0^-}^+$ Excited States of the MgNe van der Waals Molecule," *Chem. Phys. Lett.* 301, 325-330 (1999).

P.E. Curves
MgNe($^3\Pi$,$^3\Sigma$)
Excited States
Calculations

80749. McCarthy, M.C., J.W.R. Allington and K.S. Griffith, "An Accurate ab Initio Calculation of the Electron Affinity of NO," *Chem. Phys. Lett.* 289, 156-159 (1998).

P.E. Curves
NO,NO^-
Spectral Constants
EA

(80594) P.E. Curves, MPI, NaK^+, Na^+ Channels, Pathway Control, fs Pump/Probe — NaK,NaK^+

80750. Tan, H., M. Liao, D. Dai and K. Balasubramanian, "Potential Energy Surfaces of NbCO," *Chem. Phys. Lett.* 297, 173-180 (1998). — P.E. Surfaces, NbCO, Low-lying States, D_0

80751. Chen, E.C.M., and E.S. Chen, "Characterization of Homonuclear Diatomic Ions by Semiempirical Morse Potential Energy Curves. III. Rare Gas Positive Ions Revisited," *Chem. Phys. Lett.* 293, 491-498 (1998). — P.E. Curves, Ne_2^+,Ar_2^+, Kr_2^+,Xe_2^+, Morse Parameters, D_0,ω_e,r_e

80752. Ishida, T., and G.C. Schatz, "Monte Carlo Sampling Methods for Determining Potential Energy Surfaces Using Shepard Interpolation: The $O(^1D) + H_2$ System," *Chem. Phys. Lett.* 298, 285-292 (1998). — P.E. Surface, $O(^1D) + H_2$, Method

80753. Tan, H., M. Liao and K. Balasubramanian, "Potential Energy Surfaces of OsCO," *Chem. Phys. Lett.* 290, 458-464 (1998). — P.E. Surface, OsCO, Low-lying States, Interactions

80754. Nemukhin, A.V., B.L. Grigorenko and A.A. Granovsky, "Ab Initio Potential Curves of the Fragments and Diatomics-in-Molecules Potential Energy Surfaces for the SH···Kr Complex," *Chem. Phys. Lett.* 301, 287-296 (1999). — P.E. Curves, SH.Kr(A,X), DIM Calculation Method

80755. Cai, Z.-L, and J.P. Francois, "Theoretical Study of the Electronic Spectrum of the SiC^- Anion," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1007-1013 (1999). — P.E. Curves, SiC^-(B,A,X), SiC(X), Spectral Constants, (B-A),(B-X), Transition Probabilities, $B^2\Sigma^+$(v) Lifetimes, D_e,T_e,EA

80756. Kim, M.C., H.-S. Lee, Y.S. Lee and S.Y. Lee, "Low-lying States of Tl_2 Calculated by the Configuration Interaction Methods Based upon Relativistic Effective Core Potentials and Two-Component Spinors," *J. Chem. Phys.* 109, 9384-9390 (1998). — P.E. Curves, Tl_2, Low-lying States, Spectral Constants, D_e, Calculations

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

80757. Irikura, K.K., "Glossary of Common Terms and Abbreviations in Quantum Chemistry," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 441-454 (1998).

Structural
Calculations
Common Term
Glossary

80758. Demaison, J., A. Bouddou and L. Margules, "Ab Initio Bond Lengths," *J. de Chim. Phys.* 95, 1804-1817 (1998).

Structural
Calculations
Geometries
Bond Lengths
Methods
Review

80759. Feller, D., E.D. Glendening and W.A. de Jong, "Structures and Binding Enthalpies of $M^+(H_2O)_n$ Clusters, M=Cu, Ag, Au," *J. Chem. Phys.* 110, 1475-1491 (1999).

Structural
Calculations
$Ag^+(H_2O)_n, Au^+(H_2O)_n$
$Cu^+(H_2O)_n, n=1\text{-}4$
Geometries
Binding Energies

80760. Gutsev, G.L., P. Jena and R.J. Bartlett, "Structure and Stability of the AlX and AlX^- Species," *J. Chem. Phys.* 110, 2928-2935 (1999).

Structural
Calculations
AlX, AlX^-
X=H,Li,Be,B,
C,N,O,F
Low-lying States
Spectral Constants
D_0,EA

80761. Archibong, E.F., and A. St-Amant, "On the Structure of Al_2O_3 and Photoelectron Spectra of $Al_2O_2^-$ and $Al_2O_3^-$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1109-1114 (1999).

Structural
Calculations
$Al_2O_2, Al_2O_2^-$
$Al_2O_3, Al_2O_3^-$
Geometries
Frequencies
EAS

80762. Lee, H.-S., Y.-K. Han, M.C. Kim, C. Bae and Y.S. Lee, "Spin-Orbit Effects Calculated by Two-Component Coupled-Cluster Methods: Test Calculations on AuH, Au_2, TlH and Tl_2," *Chem. Phys. Lett.* 293, 97-102 (1998).

Structural
Calculations
AuH, Au_2
TlH, Tl_2
D_e, r_e, ω_e

80763. Jagielska, A., R. Moszynski and L. Piela, "Ab Initio Theoretical Study of Interactions in Borazane Molecule," *J. Chem. Phys.* 110, 947-954 (1999).

Structural
Calculations
H_3BNH_3
Geometry
Frequencies
ΔH_f

80764. Boldyrev, A.I., and J. Simons, "Inversion in the Relative Stabilities of HBO and BOH Upon Ionization," *J. Chem. Phys.* 110, 3765-3768 (1999).

Structural
Calculations
BOH^+,HBO^+
Geometries
Frequencies
Stabilities

(80836) IP,EA(BrO), Geometries, Frequencies, Calculations

BrO,$BrO^{\pm}$

80765. Workman, M.A., and J.S. Francisco, "Molecular Structure and Energetics of BrO_n Radicals (Where n=1, 2 and 3)," *Chem. Phys. Lett.* 293, 65-71 (1998).

Structural
Calculations
BrO,BrO_2,BrO_3
Geometries
Frequencies
ΔH_f

80766. Pacios, L.F., and P.C. Gomez, "Ab Initio Study of BrO_3 Isomers," *Chem. Phys. Lett.* 289, 412-418 (1998).

Structural
Calculations
BrO_3
Isomers
Geometries
Frequencies
ΔH_f

80767. Gomez, P.C., and L.F. Pacios, "Bromine and Mixed Bromine Chlorine Oxides: Wave Function (CCSD(T) and MP2) versus Density Functional Theory (B3LYP) Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 739-743 (1999).

Structural
Calculations
Br_2O_2,Cl_2O_2
$BrClO_2$
Geometries
Frequencies
ΔH_f

80768. Peterson, S., D.A. Good and J.S. Francisco, "A Density Functional Study of the Structures and Energetics of CXBrO where X=H, Cl and Br," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 916-920 (1999).

Structural
Calculations
CBrClO,CBr_2O
CHBrO
Geometries
Frequencies
ΔH_f

(80575) Electron Diffraction Structure, ps Time Resolution, $CF_2I_2+h\nu$

CF_2

80769. Li, X., and J. Paldus, "Simultaneous Handling of Dynamical and Nondynamical Correlation via Reduced Multireference Coupled Cluster Method: Geometry and Harmonic Force Field of Ozone," *J. Chem. Phys.* 110, 2844-2852 (1999).

Structural
Calculations
CF_2,$^1CH_2$
O_3,H_2O
Geometry
Frequencies
Method

80770. Song, J., Y.G. Khait and M.R. Hoffmann, "A Theoretical Study of Substituted Dioxiranes: Difluorodioxirane, Fluorofluoroxydioxirane, (Fluoroimino)dioxirane and Hydrazodioxirane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 521-526 (1999).

Structural
Calculations
$CF(OF)O_2$,$CNFO_2$
$C(NH)_2O_2$
CF_2O_2,$C_2F_2O_2^+$
Geometries
Frequencies

80771. Li, Z., and J.S. Francisco, "High Level ab Initio Molecular Orbital Study of the Structures and Vibrational Spectra of CH_2Br and CH_2Br^+," *J. Chem. Phys.* 110, 817-822 (1999).

Structural
Calculations
CH_2Br
CH_2Br^+
Geometries
Frequencies
IP

80772. Papakondylis, A., and A. Mavridis, "A Theoretical Investigation of the Structure and Bonding of Diazomethane, CH_2N_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1255-1259 (1999).

Structural
Calculations
CH_2N_2
Bonding
D_0

80773. Wiberg, K.B., R.E. Stratmann and M.J. Frisch, "A Time-Dependent Density Functional Theory Study of the Electronically Excited States of Formaldehyde, Acetaldehyde and Acetone," *Chem. Phys. Lett.* 297, 60-64 (1998).

Structural
Calculations
CH_2O,CH_3CHO
$(CH_3)_2CO$
Low-lying States
Energies
DFT Method

80774. Gutsev, G.L., P. Jena and R.J. Bartlett, "Thermodynamical Stability of CH_3ONO and CH_3ONO^-: A Coupled-Cluster and Hartree-Fock Density Functional Theory Study," *J. Chem. Phys.* 110, 403-411 (1999).

Structural
Calculations
CH_3ONO
CH_3ONO^-
Geometries
Frequencies
Fragmentation
Energies

80775. Burger, H., and W. Thiel, "Vibration-Rotation Spectra of Reactive Molecules: Interplay of ab Initio Calculations and High Resolution Experimental Studies," in *Vibration-Rotational Spectroscopy and Molecular Dynamics: Advances in Quantum Chemical and Spectroscopical Studies of Molecular Structures and Dynamics*, D. Papousek, ed., 9 Contributions, 562 pp., *Advanced Ser. Phys. Chem.* 9, 56-115 (1997).

Structural
Calculations
C_2FCl,C_2F_2
$PH_2X(X=F,Cl,Br,I)$
Theory/Spectroscopy
Interactions

80776. Lee, E.P.F., and T.G. Wright, Methylcarbyne Radical, $CH_3C(X^2A'',a^4A_2)$, and the Chemiionization Reaction: $CH_3C+O \rightarrow CH_3CO^+ + e^-$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 721-726 (1999).

Structural
Calculations
$CH_3C(a,X)$
Geometries
Frequencies
ΔH_f , T_e
CH_3C+O
Chemiionization
Energetics

(80845) Isomers, Geometries, ΔH_f , Calculations

CH_3OCO^+

80777. Dibble, T.S., "Characterization of $HOCH_2CH_2O$ and Its Dissociation Pathway," *Chem. Phys. Lett.* 301, 297-302 (1999).

Structural
Calculations
$CH_2(OH)CH_2O$
2 Conformers
Stabilities
Dissociation
Energy Barrier

80778. Salpin, J.-Y., M.T. Nguyen, G. Bouchoux, P. Gerbaux and R. Flammang, "Isomerization of Acetonitrile N-Methylide $[CH_3CNCH_2]^+$ and N-Methylketenimine $[CH_3NCCH_2]^+$ Radical Cations in the Gas Phase: Theoretical Study of the $[C_3,H_5,N]^+$ Potential Energy Surface," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 938-946 (1999).

Structural
Calculations
$C_3H_5N^+$
Isomers
$CH_3CNCH_2^+$/
$CH_3NCCH_2^+$
Isomerization
Energies,IPS

80779. Nguyen, M.T., S. Creve and T.-K. Ha, "On the Formation of the $CH_2CH_2CH=NH_2^+$ Distonic Radical Cation Upon Ionization of Cyclopropylamine and Allylamine," *Chem. Phys. Lett.* 293, 90-96 (1998).

Structural
Calculations
c-$C_3H_5NH_2^+$
$C_3H_5NH_2$
Isomers
Energies

80780. Bacskay, G.B., M. Martoprawiro and J.C. Mackie, "An ab Initio Quantum Chemical Study of the Electronic Structure and Stability of the Pyrrolyl Radical: Comparison with the Isoelectronic Cyclopentadienyl Radical," *Chem. Phys. Lett.* 290, 391-398 (1998).

Structural
Calculations
c-C_4H_4N
ΔH_f
c-C_4H_4NH
Dissociation
Mechanism

80781. Adamo, C., R. Subra, A. Di Matteo and V. Barone, "Structure and Magnetic Properties of Benzyl, Anilino and Phenoxyl Radicals by Density Functional Computations," *J. Chem. Phys.* 109, 10244-10254 (1998).

Structural
Calculations
$C_6H_5CH_2$, C_6H_5O
C_6H_5NH
Geometries
Frequencies

80782. Winkler, B., and V. Milman, "Structure and Properties of Supercubane from Density Functional Calculations," *Chem. Phys. Lett.* 293, 284-288 (1998).

Structural Calculations
Supercubane Carbon Geometry

80783. Breidung, J., W. Thiel, J. Gauss and J.F. Stanton, "Anharmonic Force Fields from Analytic CCSD(T) Second Derivatives: HOF and F_2O," *J. Chem. Phys.* 110, 3687-3696 (1999).

Structural Calculations
F_2O
HOF
Geometries
Frequencies

80784. Xu, X., X. Lu, N. Wang, Q. Zhang, M. Ehara and H. Nakatsuji, "CASSCF Study of Bonding in NiCO and FeCO," *Int. J. Quantum Chem.* 72, 221-231 (1999).

Structural Calculations
FeCO
NiCO
Electronic Bonding

80785. Gonzalez-Blanco, O., and V. Branchadell, "Density Functional Study of the Fe-CO Bond Dissociation Energies of $Fe(CO)_5$," *J. Chem. Phys.* 110, 778-783 (1999).

Structural Calculations
$Fe(CO)_5$
Geometries
Frequencies
Bond Strengths

80786. Chuang, Y.-Y., and D.G. Truhlar, "Geometry Optimization with an Infinite Basis Set," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 651-652 (1999).

Structural Calculations
H_2O, H_2O_2, NH_3
Geometry Optimization
Extrapolation Method

(80868) Chemical Bonding Calculations, D_e, r_e, Gas to Solid States

KrF_2, KrF_4, RnF_2
XeF_2, XeF_4
$XeCl_2, XeBr_2$

80787. Fuentealba, P., "On the Ground State Structure of XBO(X=Li, Na and K) Molecules," *Chem. Phys. Lett.* 301, 59-63 (1999).

Structural Calculations
LiBO,NaBO
KBO
Geometries
Frequencies

80788. Kalemos, A., A. Mavridis and S.S. Xantheas, "Theoretical Investigation of the Ground $X^3\Sigma^-$ State of Nitrogen Bromide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10536-10539 (1998).

Structural Calculations
NBr(X)
Spectral Constants
D_e(NBr,NI)

80789. Fleischer, H., and D.C. McKean, "Ab Initio Studies of Disilazanes: Structures and Vibrational Properties of Hexachloro-, Hexamethyl- and Tetrachlorodisilazane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 727-738 (1999).

Structural Calculations
$NH(SiCl_3)_2$
$NH(SiMe_3)_2$
Geometries
Frequencies

(80872) Structural Calculations, $\Delta H_f(NaO_2, NaO_2^+)$, IP($NaO_2$)

NaO_2, NaO_2^+

(80873) Structural Calculations, Geometries, Frequencies, Dissociation Energy Measurements

$Ni^+(H_2)_n$, n=1-6

80790. Muller, T., S.S. Xantheas, H. Dachsel, R.J. Harrison, J. Nieplocha, R. Shepard, G.S. Kedziora and H. Lischka, "A Systematic ab Initio Investigation of the Open and Ring Structures of Ozone," *Chem. Phys. Lett.* 293, 72-80 (1998).

Structural Calculations
O_3
Isomers
Geometries
Energies

80791. Shao, G.-Q., and W.-H. Fang, "Equilibrium Geometry of the HCCP Triplet Ground State: Phospho-Carbene, Phospho-Allene or Phosphorene? A Combined Density Functional and ab Initio Study," *Chem. Phys. Lett.* 290, 193-198 (1998).

Structural Calculations
PCCH
Frequencies
Discrepancies

80792. Fan, H.-J., and C.-W. Liu, "Ab Initio and DFT Studies on the Structure and Binding Interaction of M^+CO_2(M=Sc, Ti, ..., Zn)," *Chem. Phys. Lett.* 300, 351-358 (1999).

Structural Calculations
Sc^+CO_2 thru Zn^+CO_2
Geometries
Binding Energies

80793. Koput, J., S. Carter and N.C. Handy, "The Vibrational-Rotational Energy Levels of Silanone," *Chem. Phys. Lett.* 301, 1-9 (1999).

Structural Calculations
$Si(H_2)O$
P.E. Surface
Frequencies
v,J Energy Levels

80794. Cai, Z.-L., and J.P. Francois, "Ab Initio Study of the Lowest $^3\Sigma^-$, $^3\Pi$ and $^1\Sigma^+$ States of the SiN^+ Cation," *Chem. Phys. Lett.* 300, 69-79 (1999).

Structural Calculations
$SiN^+(^1\Sigma^+, ^3\Pi, X^3\Sigma^-)$
Spectral Constants
T_0, D_0

80795. Solomonik, V.G., J.E. Boggs and J.F. Stanton, "Jahn-Teller Effect in VF_3," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 838-840 (1999).

Structural Calculations
$VF_3(^3A_2', X^3E'')$
Geometry
Jahn-Teller Distortions

(80876) Geometries, DFT Calculations, D, IPS

V_n, V_n^+, n=2-9

45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

80796. Allcock, P., R.D. Jenkins and D.L. Andrews, "Laser Assisted Resonance Energy Transfer," *Chem. Phys. Lett.* 301, 228-234 (1999).

Energy Transfer
Electronic
Long Range
Laser Assisted
Theory

80797. Gorling, C., E. Jalviste, N. Ohta and C. Ottinger, "Lifetime Measurements of the Collision-Free Slow Fluorescence from Glyoxal S_1/T_1 Gateway Levels in a Beam," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10620-10629 (1998).

Energy Transfer
$(CHO)_2, S_1/T_1$
Gateway Levels
Fluorescence
Decay Times

80798. Clegg, S.M., B.D. Gilbert, S.-p. Lu and C.S. Parmenter, "Crossed Molecular Beam Observations of Vibrational Energy Transfer in Only Moderately Excited Glyoxal Molecules," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 237-250 (1997).

E-R,V-R
Relaxation
$(CHO)_2, (S_1) + M$
Cross Sections
$M = CO, C_2H_4, D_2, N_2$

(80664) Excited Singlet State, P.E. Surfaces, Efficient Relaxation Channel

$CH_2(CHO)_2$*

80799. Raab, A., G.A. Worth, H.-D. Meyer and L.S. Cederbaum, "Molecular Dynamics of Pyrazine after Excitation to the S_2 Electronic State Using a Realistic 24-Mode Model Hamiltonian," *J. Chem. Phys.* 110, 936-946 (1999).

Energy Relaxation
c-$C_4H_4N_2(S_2)$
P.E. Surfaces
Mode Coupling
Calculations

80800. Kaledin, A.L., M.C. Heaven and K. Morokuma, "Ab Initio Potential Energy Surfaces for the $I(^2P_{3/2}) + O_2(a^1\Delta_g) \leftrightarrow I(^2P_{1/2}) + O_2(X^3\Sigma_g^-)$ Energy Transfer Process," *Chem. Phys. Lett.* 289, 110-117 (1998).

E-E Transfer
$O_2(a) + I/$
$O_2 + I(^2P_{1/2})$
P.E. Surface
Crossings

80801. Gimelshein, S.F., M.S. Ivanov, G.N. Markelov and Yu.E. Gorbachev, "Statistical Simulation of Nonequilibrium Rarefied Flows with Quasiclassical Vibrational Energy Transfer Models," Presented Originally as AIAA Paper 97-2585 at the *32nd AIAA Thermophysics Conference,* Held in Atlanta GA, June 1997, *J. Thermophys. Heat Transfer* 12, 489-495 (1998).

V-V-T
Energy Exchange
Models
Nonequilibrium
Flow
Simulations

(80620) Effects on Unimolecular Isomerization, Model

IVR

80802. Bigwood, R., M. Gruebele, D.M. Leitner and P.G. Wolynes, "The Vibrational Energy Flow Transition in Organic Molecules: Theory Meets Experiment," *Proc. Nat. Acad. Sci. USA* 95, 5960-5964 (1998).

Vibrational
Energy Transfer
Organics
Overview

(80383) Laser Spectroscopy, Highly Sensitive, $CHCl_3$, CS_2, OCS, C_2H_2, C_2H_4, H_2S, Methods, Review

IVR,Overtones

80803. Perry, D.S., "Time Scales and Mechanisms of Intramolecular Energy Redistribution," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 70-80 (1997).

IVR
CHF_3,CF_2Cl_2
C_2H_5OH,C_4H_6
Timescales
Overview

80804. Pino, G.A., C.A. Rinaldi, E.A. Coronado and J.C. Ferrero, "Collisional Relaxation of Highly Vibrationally Excited CF_2O Prepared with Different Initial Energies and Distribution Functions," *J. Chem. Phys.* 110, 1942-1948 (1999).

Vibrational Relaxation
$COF_2(v)+M$
Average Energy Transfers
Initial Distribution Independence

80805. Lendvay, G., G.C. Schatz and T. Takayanagi, "Quantum Scattering Studies of Collisional Energy Transfer from Highly Excited Polyatomic Molecules: Colinear $He+CS_2$ at Energies up to 92 kcal/mol," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 202-219 (1997).

Energy Transfer
CS_2+He
$\leq$92 kcal mol^{-1}
Average Value Probabilities
Calculations

80806. Bradley, K.S., G.C. Schatz and G.G. Balint-Kurti, "Wavepacket Methods for the Direct Calculation of Energy Transfer Moments in Molecular Collisions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 947-952 (1999).

Energy Transfer
CS_2+He
H_2+He
Wavepacket Theory

80807. Green, D., S. Hammond, J. Keske and B.H. Pate, "Intramolecular Vibrational Energy Redistribution and Conformational Isomerization in Vibrationally Excited 2-Fluoroethanol: High Resolution, Microwave-Infrared Double-Resolution Spectroscopy Investigation of the Asymmetric-CH_2(F) Stretch Near 2980 cm^{-1}," *J. Chem. Phys.* 110, 1979-1989 (1999).

IVR
CH_2FCH_2OH
–CH_2(F) Stretch
Lifetime
Isomerization
Measurements

(80708) Vibrational Energy Distributions, Polyatomics, Decay Rate Interpretation, New Method

c-$C_4H_4N_2$

80808. Minehardt, T.J., J.D. Adcock and R.E. Wyatt, "Quantum Dynamics of Overtone Relaxation in 30-Mode Benzene: A Time-Dependent Local Mode Analysis for CH($v=2$)," *J. Chem. Phys.* 110, 3326-3334 (1999).

Energy Transfer
$C_6H_6(2\nu_{CH})$
Flow Modes
Modeling

80809. Rashev, S., "A Quantum Mechanical Study of the Role of Out-of-Plane Vibrations in Benzene in the Intramolecular Redistribution of Vibrational Energy," *J. Chem. Phys.* 110, 2489-2497 (1999).

IVR
$C_6H_6(3\nu_{CH})$
Level Mixing
Calculations

80810. Gruebele, M., "Intramolecular Vibrational Dephasing Obeys a Power Law at Intermediate Times," *Proc. Nat. Acad. Sci. USA* 95, 5965-5970 (1998).

IVR
$C_{13}H_{10}$,$C_{14}H_{10}$
$C_6H_5NHC_6H_{11}$
Power Law Decays

(80608) Vibrational Relaxation Rate Constant, $Cl+O_3$, $ClO(v,J,\Lambda)$ Product Distributions

$ClO(v)+N_2$

(80418) V,R Energy Transfer Cross Sections, $v'=7$, $J'=6$, LIF Measurements

KH(A),v,J

(80338) Supersonic Air, Nozzle Flow

NO Formation
Nonequilibrium
Relaxation Effects

(80339) Hypersonic Flows, Zeldovich Mechanism

NO Formation
Nonequilibrium
Relaxation Effects

80811. Drabbels, M., and A.M. Wodtke, "Infrared and Collisional Relaxation of Highly Vibrationally Excited NO: Applications of Stimulated Emission Pumping in Crossed and 'Uncrossed' Molecular Beams," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 173-190 (1997).

Vibrational
Rotational
Relaxation
$NO(v=20,J=0.5)+He$
$NO(v=20\text{-}22)+N_2O$
Cross Sections
NO(v) Infrared
A-Factors

80812. Dai, H.-L., "Collisional Energy Transfer of Highly Vibrationally Excited Molecules: The Role of Long-Range Interaction and Intramolecular Vibronic Coupling," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, A.S. Mullin and G.C. Schatz, eds., 21 Papers, 330 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 678, 266-274 (1997).

V-V,V-T/R
NO_2
Highly Excited
Long Range
Energy Transfer

80813. Abel, B., N. Lange, F. Reiche and J. Troe, "State-Resolved Collisional Energy Transfer in Highly Excited NO_2. I. Cross Sections and Propensities for J, K, and m_J Changing Collisions," *J. Chem. Phys.* 110, 1389-1403 (1999).

Energy Transfer
$NO_2(v,J)+NO_2$
State-to-State
Cross Sections
Propensity
Patterns

80814. Abel, B., N. Lange, F. Reiche and J. Troe, "State-Resolved Collisional Energy Transfer in Highly Excited NO_2. II. Vibrational Energy Transfer in the Presence of Strong Chemical Interaction," *J. Chem. Phys.* 110, 1404-1415 (1999).

Vibrational
Relaxation
$NO_2(v)+NO_2$
Cross Sections

80815. Yamasaki, K., A. Watanabe, T. Kakuda, N. Ichikawa and I. Tokue, "First Determination of the Branching Ratios between Reactive Removal and Vibrational Relaxation in Collisions of OH($X^2\Pi_i$, v=1 and 2) with CH_4" *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 451-459 (1999).

Vibrational Relaxation
$OH(v=1,2)+CH_4$
Reactive Channel
Branching Ratios
Rate Constants

80816. Campos-Martinez, J., E. Carmona-Novillo, J. Echave, M.I. Hernandez, R. Hernandez-Lamoneda and J. Palma, "Jump in Depletion Rates of Highly Excited O_2: Reaction or Enhanced Vibrational Relaxation?," *Chem. Phys. Lett.* 289, 150-155 (1998).

Vibrational Relaxation
$O_2(v)+O_2$
Enhanced Rates
Nonreactive

(80696) Dominance of Vibrational Relaxation over Reaction, Channels, Rate Constants, Calculations

$O_2(v\gg0)+O_2$

(80456) Relaxation Rate Constants, M=CO, H_2,NO, N_2

$PH_2(X,v=1)+M$
$PH_2(A,v=1,0)+M$

80817. Vallance, C., W.-P. Hu and P.W. Harland, "Upper Stark State Collisional Relaxation Cross Sections for Single Rotational States of CH_3F," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 665-670 (1999).

ΔM Relaxation
CH_3F+Ar
Stark Split
Cross Sections

80818. Yang, X., and P.J. Dagdigian, "Selective Rotational Energy Transfer from Individual Λ-Doublet Levels of Highly Rotational Excited CN($A^2\Pi$)," *Chem. Phys. Lett.* 297, 506-514 (1998).

Rotational Energy Transfer
$CN(A,v=3,N=60)+Ar$
Fine Structure
Rate Constants

80819. Antonova, S., A. Lin, A.P. Tsakotellis and G.C. McBane, "State-to-State He-CO Rotational Inelastic Scattering," *J. Chem. Phys.* 110, 2384-2390 (1999).

Rotational Energy Transfer
$CO(J)+He$
Cross Sections

80820. Ahern, M.M., D.A. Steinhurst and M.A. Smith, "Rotational Relaxation of CO in He, Ar, N_2 and CO Free Jets," *Chem. Phys. Lett.* 300, 681-686 (1999).

Rotational Relaxation
CO(J)
Distributions
$CO/CO,He,Ar,N_2$
Free Jets
REMPI Probe

80821. Lin, A., S. Antonova, A.P. Tsakotellis and G.C. McBane, "Λ Doublet Propensities in Ar-NO Rotationally Inelastic Scattering at 220 meV," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1198-1205 (1999).

Rotational Energy Transfer
$NO+Ar$
Λ Doublet
Propensities
Cross Sections

80822. Ball, C.D., and F.C. De Lucia, "Direct Observation of Λ-Doublet and Hyperfine Branching Ratios for Rotationally Inelastic Collisions of NO-He at 4.2 K," *Chem. Phys. Lett.* 300, 227-235 (1999).

Energy Transfer
NO+He
4.2 K Measurements
Propensities

80823. Aoiz, F.J., T. Diez-Rojo, V.J. Herrero, B. Martinez-Haya, M. Menendez, P. Quintana, L. Ramonat, I. Tanarro and E. Verdasco, "Low Temperature Rotational Relaxation of N_2 Studied with Resonance Enhanced Multiphoton Ionization," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 823-832 (1999).

Rotational
Relaxation
N_2
Cross Sections
Low Temperatures

80824. Kliner, D.A.V., and R.L. Farrow, "Measurements of Ground State OH Rotational Energy Transfer Rates," *J. Chem. Phys.* 110, 412-422 (1999).

Rotational
Energy Transfer
OH(X,v,N)+M
Rate Constants
$M = Ar, H_2O, N_2, O_2$
Exponential
Gap Model

46. THERMOCHEMISTRY

80825. Frurip, D.J., and J.W. Storer, "Appendix A: Software and Databases for Thermochemistry," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 384-401 (1998).

Thermochemistry
Databases
Software
Availability
Review

80826. Irikura, K.K., and D.J. Frurip, "Computational Thermochemistry," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 2-18 (1998).

Thermochemical
Data
Calculation
Methods
Overview

80827. Benson, S.W., and N. Cohen, "Current Status of Group Additivity," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 20-46 (1998).

Thermochemical
Data
Group Additivity
Current Status

80828. Zachariah, M.R., and C.F. Melius, "Bond-Additivity Correction of ab Initio Computations for Accurate Prediction of Thermochemistry," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 162-175 (1998).

Thermochemical
Data
Calculations
Bond Additivity
Correction Method

80829. Irikura, K.K., and D.J. Frurip, "Appendix C: Worked Examples," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 419-440 (1998).

ΔH_f
Calculation Methods
Examples

80830. Irikura, K.K., "Appendix B: Essential Statistical Thermodynamics," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 402-418 (1998).

Statistical Thermodynamics
C_p,$S°$,H_T-H_0
Calculation Methods

80831. Petersson, G.A., D.K. Malick, W.G. Wilson, J.W. Ochterski, J.A. Montgomery Jr and M.J. Frisch, "Calibration and Comparison of the Gaussian-2, Complete Basis Set, and Density Functional Methods for Computational Thermochemistry," *J. Chem. Phys.* 109, 10570-10579 (1998).

ΔH_f
Large Molecular Set
Theoretical Methods
Comparisons
Accuracies

(80760) X=H, Li, Be, B, C, N, O, F, Structural Calculations, Low-lying States, Spectral Constants

$D_0(AlX,AlX^-)$
EA(AlX)

(80761) Structural Calculations, Geometries, Frequencies

EA(Al_2O_2 ,Al_2O_3)

(80736) P.E. Curves, Spectral Constants, Energy Levels, Calculations

$D_0(Ar_2(B,X))$

80832. Lippa, T.P., S.-J. Xu, S.A. Lyapustina, J.M. Nilles and K.H. Bowen, "Photoelectron Spectroscopy of As^-, As_2^-, As_3^-, As_4^- and As_5^-," *J. Chem. Phys.* 109, 10727-10731 (1998).

EA(As_n)
n=1-5
As_2^-
Spectral Constants
D_0 ,S/O Splitting

80833. Lippa, T.P., S.-J. Xu, S.A. Lyapustina and K.H. Bowen, "Negative Ion Photoelectron Spectroscopy of the AsO^- Anion," *J. Chem. Phys.* 109, 9263-9265 (1998).

D(AsO^-)
PES Spectra
Constants
(a/X) Splitting
EA(AsO)

(80762) Structural Calculations, r_e , ω_e

$D_e(AuH,Au_2)$
$D_e(TlH,Tl_2)$

80834. Politzer, P., P. Lane and M.C. Concha, "Computational Determination of the Energetics of Boron Ignition/Combustion Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1419-1425 (1999).

ΔH_f
B/H/C/O/F
Molecules
B Ignition Reactions
$\Delta H_{Reaction}$

80835. Godefroy, P., J.M. Vierfond and J.P. Vantelon, "Vaporization of a Pyrophoric Substance: Borane Triethyl," *J. Fire Sci.* 16, 159-178 (1998).

$BH(C_2H_5)_3$,(l)
Vaporization
Properties

(80763)	Structural Calculations, Geometry, Frequencies	$\Delta H_f(H_3BNH_3)$
80836.	Francisco, J.S., S. Parthiban and T.J Lee, "Adiabatic Electron Affinity and Ionization Potential for BrO Radical," *J. Chem. Phys.* 109, 10818-10822 (1998).	IP,EA(BrO) Neutral,Ions Geometries Frequencies Calculations
(80765)	Structural Calculations, Geometries, Frequencies	$\Delta H_f(BrO,BrO_2)$ $\Delta H_f(BrO_3)$
(80766)	Isomers, Structural Calculations, Geometries, Frequencies	$\Delta H_f(BrO_3)$
(80767)	Structural Calculations, Geometries, Frequencies	$\Delta H_f(Br_2O_2, Cl_2O_2)$ $\Delta H_f(BrClO_2)$
80837.	Marshall, P., A. Misra and M. Schwartz, "A Computational Study of the Enthalpies of Formation of Halomethylidynes," *J. Chem. Phys.* 110, 2069-2073 (1999).	ΔH_f(CBr,CCl,CF) ΔH_f(CH,CI) Calculations
(80768)	Structural Calculations, Geometries, Frequencies	$\Delta H_f(CBrClO,CBr_2O)$ ΔH_f(CHBrO)
80838.	Ruscic, B., J.V. Michael, P.C. Redfern, L.A. Curtiss and K. Raghavachari, "Simultaneous Adjustment of Experimentally Based Enthalpies of Formation of CF_3X (X=nil, H, Cl, Br, I, CF_3, CN) and a Probe of G3 Theory," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10889-10899 (1998).	ΔH_f (CF_3,CF_3X) X=CF_3,CN,Cl,Br,I,H IP(CF_3),$\Delta H_f(C_2F_4)$ Calculations
80839.	Berry, R.J., M. Schwartz and P. Marshall, "Ab Initio Calculations for Kinetic Modeling of Halocarbons," in *Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics*, K.K. Irikura and D.J. Frurip, eds., 24 Papers, 470 pp., Presented at the *212th National Meeting of the American Chemical Society*, Held in Orlando FL, August 1996, *Am. Chem. Soc. Symposium Ser.* 677, 341-358 (1998).	ΔH_f CH_nX_{4-n},$CH_nF_mCl_p$ $C_2H_nF_{6-n}$,$C_2H_nF_{4-n}$ H,OH Reaction Energies Calculations
80840.	Li, X., and J. Paldus, "Singlet-Triplet Splitting in Methylene: An Accurate Description of Dynamic and Nondynamic Correlation by Reduced Multireference Coupled Cluster Method," *Collect. Czech. Chem. Commun.* 63, 1381-1393 (1998).	$^{1,3}CH_2$ Energy Splitting Calculations
(80771)	Structural Calculations, CH_2Br, CH_2Br^+, Geometries, Frequencies	IP(CH_2Br)
(80772)	Structural Calculations, Bonding	$D_0(CH_2N_2)$
80841.	Franscisco, J.S., and J.W. Thoman Jr, "Adiabatic Ionization Potential and Electron Affinity of Formaldehyde," *Chem. Phys. Lett.* 300, 553-560 (1999).	IP,EA(CH_2O) Calculations
(80604)	$CH_3I + hv$, Product 2-D Energy Mapping, $CH_3(T,v,J)$, $I(^2P_{1/2,3/2})$, Dynamics	D(CH_3I)

80842.	Messer, B.M., and M.J. Elrod, "A Theoretical Study of ROX (R=H,CH_3; X=F,Cl,Br) Enthalpies of Formation, Ionization Potentials and Fluoride Affinities," *Chem. Phys. Lett.* 301, 10-18 (1999).	ΔH_f ,IP,FA CH_3OF,CH_3OCl,CH_3OBr HOF,HOCl,HOBr Calculations
(80578)	CH_3S, $CD_3S+h\nu$, $CH_3(v)$, $S(^3P_J)$ Product Distributions, Predissociation	$\Delta H_f(CH_3S)$
80843.	Signorell, R., and F. Merkt, "The First Rotationally Resolved Spectrum of CH_4^+," *J. Chem. Phys.* 110, 2309-2311 (1999).	IP(CH_4,CD_4) PFI/ZEKE Spectra
(80740)	P.E. Curves, Low-lying States, Ultraviolet and Photoelectron Spectral Assignments, COF_2^+ Frequencies, Calculations	IP(COF_2)
(80509)	$CH_4/O_2/C_2HCl_3$ Flame Sampling, Mass Analysis	IP(CCl_2CHOH)
80844.	Nguyen, T.L., and M.T. Nguyen, "On the Heats of Formation of Formyl Cyanide and Thioformyl Cyanide," *J. Chem. Phys.* 110, 684-686 (1999).	$\Delta H_f(CH(O)CN)$ $\Delta H_f(CH(S)CN)$ Calculations
(80528)	Shock Tube Pyrolysis CH_3CN/Ar, Products, Rate Constants, Kinetic Modeling	$\Delta H_f(CH_2CN)$
(80776)	Structural Calculations, Geometries, Frequencies, T_e	$\Delta H_f(CH_3C(a,X))$
(80552)	CH_3CCl_2, CH_3CBr_2+Br Reaction Rate Constants, Temperature Dependences, Measurements	$\Delta H_f(CH_3CCl_2)$ $\Delta H_f(CH_3CBr_2)$
80845.	Ruttink, P.J.A., P.C. Burgers, L.M. Fell and J.K. Terlouw, "G2 Theory and Experiment in Concert: Enthalpy of Formation of CH_3O-C=O^+ and Its isomers Revisited," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1426-1431 (1999).	$\Delta H_f(CH_3OCO^+)$ Isomers Geometries Calculations
(80663)	Calculations	$\Delta H_f(CH_3OCH_2)$ $\Delta H_f(CH_3OCH_2O_2)$ $\Delta H_f(CH_2OCH_2OOH)$
(80707)	TNAZ Thermal Dissociation, FT Mass Analysis, Also Product IPS	IP($C_3H_4N(NO_2)_3$)
80846.	Nguyen, M.T., and H.M.T. Nguyen, "On the Heats of Formation of Methylketene, Dimethylketene and Related Cations," *Chem. Phys. Lett.* 300, 346-350 (1999).	ΔH_f CH_3CHCO,CH_3CHCO^+ $(CH_3)_2CCO$,$(CH_3)_2CCO^+$ $C_2H_5CO^+$,$(CH_3)_2CHCO^+$ Calculations
(80778)	Structural Calculations, $C_3H_5N^+$ Isomers, IPS, Isomerization Energies, Fragmentations	$\Delta H_f(CH_3CNCH_2^+)$ $\Delta H_f(CH_3NCCH_2^+)$
(80633)	Unimolecular Isomerization, $C_2H_5COOCH_3^+$, Channels, Measurements	$\Delta H_f(C_2H_5CO^+)$ IP($C_2H_5COOCH_3$)
(80780)	Structural Calculations	ΔH_f(*c*-C_4H_4N)

80847. Smith, B.J., and L. Radom, "Heat of Formation of the *tert*-Butyl Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10787-10790 (1998).

ΔH_f,IP(*t*-C_4H_9)
ΔH_f(*i*-$C_4H_8^+$,*t*-$C_4H_9^+$)
Calculations

80848. Clifford, E.P., P.G. Wenthold, R. Gareyev, W.C. Lineberger, C.H. DePuy, V.M. Bierbaum and G.B. Ellison, "Photoelectron Spectroscopy, Gas Phase Acidity, and Thermochemistry of *tert*-Butyl Hydroperoxide: Mechanisms for the Rearrangement of Peroxyl Radicals," *J. Chem. Phys.* 109, 10293-10310 (1998).

EA(*t*-$C_4H_9O_2$)
EA(HO_2)
D(*t*-C_4H_9OOH)
Ion Photoelectron Spectra
A/X State Energy Gaps

(80533) Shock Tube Pyrolysis *c*-C_5H_6/Ne, Rate Constants, RRKM Analysis

ΔH_f(*c*-C_5H_5)

80849. Segovia, J.J., M.C. Martin, C.R. Chamorro and M.A. Villamanan, "Thermodynamics of Octane-Enhancing Additives in Gasolines: Vapor-Liquid Equilibrium of the Ternary Mixtures Methyl *tert*-Butyl Ether + Heptane + Benzene and Methyl *tert*-Butyl Ether + Benzene + 1-Hexene at 313.15 K," *J. Chem. Eng. Data* 43, 1014-1020 (1998).

Vapor Pressures
C_6H_6/C_7H_{16}/(M)
C_6H_6/C_6H_{12}/(M)
M = *t*-$C_4H_9OCH_3$
Binary/Ternary Mixture Behavior

80850. Segovia, J.J., M.C. Martin, C.R. Chamorro and M.A. Villamanan, "Vapor-Liquid Equilibrium of Ternary Mixtures Containing Methyl *tert*-Butyl Ether and/or Substitution Hydrocarbons: Methyl *tert*-Butyl Ether + Heptane + Cyclohexane and Methyl *tert*-Butyl Ether + Cyclohexane + 1-Hexene at 313.15 K," *J. Chem. Eng. Data* 43, 1021-1026 (1998).

Vapor Pressures
c-C_6H_{12}/C_7H_{16}/(M)
c-C_6H_{12}/C_6H_{12}/(M)
M = *t*-$C_4H_9OCH_3$
Binary/Ternary Mixture Behavior

80851. Lazarou, Y.G., and P. Papagiannakopoulos, " Theoretical Investigation of the Thermochemistry of Hydrofluoroethers," *Chem. Phys. Lett.* 301, 19-28 (1999).

ΔH_f
19 Fluoroethers
Radicals
Fluoroethanes
Calculations

80852. Orlov, Yu.D., R.K. Zaripov and Yu.A. Lebedev, "Determination of Enthalpies of Formation of Organic Free Radicals from Bond Dissociation Energies. II. Halosubstituted Radicals," *Russ. Chem. Bull.* 47, 621-624 (1998).

ΔH_f
23 Haloorganic Radicals
D(RX)
Estimation Method

80853. Jursic, B.S., "Reliability of Hybrid Density Theory: Semiempirical Approach for Evaluation of Bond Dissociation Energies," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 369-372 (1999).

D(RH)
D(RR′)
Organics
Estimation Method

80854. Hammerum, S., "Heats of Formation and Proton Affinities by the G3 Method," *Chem. Phys. Lett.* 300, 529-532 (1999).

ΔH_f,PA
29 Organics
G3 Method
Accuracies

80855. Oja, V., and E.M. Suuberg, "Vapor Pressures and Enthalpies of Sublimation of Polycyclic Aromatic Hydrocarbons and Their Derivatives," *J. Chem. Eng. Data* 43, 486-492 (1998).

$\Delta H_{Sublimation}$
Vapor Pressures
8 PAHS
7 Heteroatom PAHS

80856. Orlov, Yu.D., R.K. Zaripov and Yu.A. Lebedev, "Determination of Enthalpies of Formation of Organic Free Radicals from Bond Dissociation Energies. I. Hydrocarbon Radicals," *Russ. Chem. Bull.* 47, 615-620 (1998).

ΔH_f
24 Hydrocarbon PAH Radicals
Macroincrement Estimation Method

80857. Barckholtz, C., T.A. Barckholtz and C.M. Hadad, "C-H and N-H Bond Dissociation Energies of Small Aromatic Hydrocarbons," *J. Am. Chem. Soc.* 121, 491-500 (1999).

D
Aromatics
PAHS
Computational Methods
Accuracies

80858. Zhogova, K.B., and B.V. Lebedev, "Thermodynamics of C_{70} Fullerene in the 0-390 K Temperature Range," *Russ. Chem. Bull.* 47, 625-628 (1998).

$C_{70}(s)$
Thermodynamic Values
fef, $S°$, H_T-H_0
ΔH_f, ΔG_f, ΔS_f
Measurements

80859. Oja, V., and E.M. Suuberg, "Measurements of the Vapor Pressures of Coal Tars Using the Nonisothermal Knudsen Effusion Method," *Energy Fuels* 12, 1313-1321 (1998).

Vapor Pressures
Primary
Coal Tars
Measurements

80860. Cacace, F., G. de Petris, F. Pepi, M. Rosi and A. Sgamellotti, "Elemental Chlorine and Chlorine Fluoride: Theoretical and Experimental Proton Affinity and the Gas Phase Chemistry of Cl_2H^+ and $FClH^+$ Ions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10560-10567 (1998).

PA(Cl_2, FCl)
Measurements
Calculations

(80407) Spectral Constants, Calculations

$D_0(Cr_2)$

(80741) P.E. Curves, Low-lying States, Spectral Constants, Energies, Calculations

D_e(CsHg)

80861. Ventura, O.N., R.E. Cachau and M. Kieninger, "Density Functional and Coupled-Cluster Calculations of Isodesmic Reactions Involving Fluorine Oxides," *Chem. Phys. Lett.* 301, 331-335 (1999).

ΔH_f(FO)
Calculations

80862. Ventura, O.N., M. Kieninger and R.E. Cachau, "Density Functional Theory is More Accurate Than Coupled-Cluster Theory in the Study of the Thermochemistry of Species Containing the F-O Bond," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 147-151 (1999).

$\Delta H_f(FO,FO_2)$
$\Delta H_f(FOH,F_2O)$
Calculations
Accuracies

80863. Kellogg, C.B., and K.K. Irikura, "Gas Phase Thermochemistry of Iron Oxides and Hydroxides: Portrait of a Super-Efficient Flame Suppressant," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 1150-1159 (1999).

ΔH_f
FeH,FeO,FeOH
FeO_2,FeO(OH),$Fe(OH)_2$
Flame Suppression
Reaction Energies

80864. Bauschlicher Jr, C.W., C.F. Melius and M.D. Allendorf, "Gallium Compounds, a Possible Problem for the G2 Appproaches," *J. Chem. Phys.* 110, 1879-1881 (1999).

Atomization
Energies
Ga/O/F
9 Compounds
G2 Errors
GaF_2 Values

(80743) P.E. Curves, Low-lying States, Spectral Constants, Calculations

D_0,ΔH_f(GeC)

80865. Anderson, W.R., "Heats of Formation of HNO and Some Related Species," *Combust. Flame* 117, 394-403 (1999).

ΔH_f(HNO,HNO^+)
ΔH_f(HNO^-,NO)
ΔH_f(NH_2OH)
Critical Review

80866. Thorn Jr, R.P., L.J. Stief, S.-C. Kuo and R.B. Klemm, "Photoionization Mass Spectrometric Study of HOCl: Photoionization Efficiency Spectrum and Ionization Energy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 812-815 (1999).

IP(HOCl)
ΔH_f($HOCl^+$)
PA(ClO)
Photoionization
Measurements

80867. Suleimenov, O.M., and T.-K. Ha, "Ab Initio Calculation of the Thermochemical Properties of Polysulphanes (H_2S_n)," *Chem. Phys. Lett.* 290, 451-457 (1998).

Thermochemical
Values
H_2S_n
C_p,S°,H_T-H_0
Calculations

(80539) IO+BrO Rate Constants, Measurements

ΔH_f(IO_2)

(80746) fs Photoelectron Spectrum, Pump/Probe, P.E. Curve, r_e, Measurements

D_e(I_2^-(A′))

(80747) P.E. Curves, r_e, Calculations

D_e
KrF,KrF^+
$^{1,3}KrF_2$,$Kr.F_2$

80868. Liao, M.-S., and Q.-E. Zhang, "Chemical Bonding in XeF_2, XeF_4, KrF_2, KrF_4, RnF_2, $XeCl_2$ and $XeBr_2$: From the Gas Phase to the Solid State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10647-10654 (1998).

D_e, r_e
KrF_2,KrF_4,RnF_2
XeF_2,XeF_4
$XeCl_2$,$XeBr_2$
Chemical Bonding
Calculations

80869. Sievers, M.R., and P.B. Armentrout, "Reactions of CO and CO_2 with Gas Phase Mo^+, MoO^+ and MoO_2^+," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 10754-10762 (1998).

D_0(Mo^+CO_2,MoO^+CO_2)
D(Mo^+O_2)
Guided Ion Beam
Measurements

(80788)	Structural Calculations, Spectral Constants	D_e(NBr,NI)
80870.	Ricca, A., "Accurate D_0 Value for NF^+," *Chem. Phys. Lett.* 300, 80-84 (1999).	$D_0(NF^+)$ Calculations
(80749)	P.E. Curves, NO, NO^-, Spectral Constants, Calculations	EA(NO)
80871.	Taylor, T.R., R.T. Bise, K.R. Asmis and D.M. Neumark, "The Singlet-Triplet Splittings of NCN," *Chem. Phys. Lett.* 301, 413-416 (1999).	NCN(b,a,X) Energy Spacing Anions PES b-State Frequency
(80712)	Dissociation, Channels, DFT Calculations	$\Delta H_{Reaction}$ $NH_4N(NO_2)_2$,(c)
80872.	Lee, E.P.F., P. Soldan and T.G. Wright, "The Heat of Formation of $NaO_2^+(X^3\Sigma^-)$ and $NaO_2(X^2A_2)$," *Chem. Phys. Lett.* 301, 317-324 (1999).	$\Delta H_f(NaO_2, NaO_2^+)$ $IP(NaO_2)$ Structural Calculations
(80750)	P.E. Surfaces, Low-lying States	D_0(NbCO)
(80751)	P.E. Curves, Morse Parameters, r_e, ω_e, Spectral Evaluations	$D_0(Ne_2^+, Ar_2^+)$ $D_0(Kr_2^+, Xe_2^+)$
80873.	Kemper, P.R., P. Weis and M.T. Bowers, "$Ni^+(H_2)_n$: Ligand Bond Energies for Ground State Ions," *Chem. Phys. Lett.* 293, 503-510 (1998).	$D(Ni^+(H_2)_n)$ n=1-6 Geometries Frequencies Measurements Calculations
(80569)	$Ni(a^3D_J, a^3F_J) + SO_2 + Ar$, Rate Constants, Measurements	$D(NiSO_2)$
(80428)	$O_2^+(B)$, $O_2^+(^2\Sigma_u^-)$, v′=0-7 Upper States, PFI/PES Spectra, Ion Constants, Predissociation Lifetimes	$IP(O_2)$
(80255)	Calculations	$\Delta H_f(P_2H_n^+)$,n=0-4
(80668)	$Cl^+(^1D, ^3P) + H_2S$, P.E. Surfaces, Energies, Calculations	$\Delta H_f(H_2SCl^+)$
80874.	Cheng, B.-M., and W.-C. Hung, "Photoionization Efficiency Spectrum and Ionization Energy of S_2O_2," *J. Chem. Phys.* 110, 188-191 (1999).	$IP(S_2O_2)$ Photoionization Spectrum
(80755)	P.E. Curves, Spectral Constants, Calculations	$D_e, T_e(SiC, SiC^-)$ EA(SiC)
80875.	Wenthold, P.G., "A Computational Study of the Electron Affinity of Silene," *Chem. Phys. Lett.* 297, 445-450 (1998).	EA(SiH_2CH_2) ^{1,3}Energy Splitting Calculations
(80794)	Structural Calculations, Spectral Constants, T_0	$D_0(SiN^+(^1\Sigma^+, ^3\Pi, X))$

(80257) Sn Flame Chemistry, Probe Sampling/Mass Analysis, Species Profiles, $SnOH^+ + e^-$ Rate Constant

PA(SnO)
$\Delta H_f, D_0(SnOH^+)$

(80756) P.E. Curves, Spectral Constants, Low-lying States, Calculations

$D_e(Tl_2)$

80876. Wu, X., and A.K. Ray, "A Density Functional Study of Small Neutral and Cationic Vanadium Clusters V_n and V_n^+ (n=2-9)," *J. Chem. Phys.* 110, 2437-2445 (1999).

$D(V_n, V_n^+)$
IP(V_n)
Geometries
DFT Calculations

80877. Gee, C., P. Boissel and G. Ohanessian, "Metal-Acetylene Binding in Gaseous $WC_2H_2^+$," *Chem. Phys. Lett.* 298, 85-92 (1998).

$D(WC_2H_2^+)$
Photodissociation
Measurements

80878. Sievers, M.R., and P.B. Armentrout, "Activation of Carbon Dioxide: Gas Phase Reactions of Y^+, YO^+ and YO_2^+ with CO and CO_2," *Inorganic Chem.* 38, 397-402 (1999).

$D_0(Y^+CO, OY^+CO)$
$D_0(O_2Y^+CO, OY^+CO_2)$
$Y^+, YO^+ + CO_2$
$YO^+, YO_2^+ + CO$
Ion Beam
Reaction Thresholds

47. EXPERIMENTAL METHODS

80879. Paolini, B.P., and M.A. Khakoo, "An Intense Atomic Hydrogen Source with a Movable Nozzle Output," *Rev. Sci. Instrum.* 69, 3132-3135 (1998).

H-Atom
Source
Movable Nozzle
Microwave Method

80880. Althorpe, S.C., and T. Seideman, "Molecular Alignment from Femtosecond Time-Resolved Photoelectron Angular Distributions: Nonperturbative Calculations on NO," *J. Chem. Phys.* 110, 147-155 (1999).

NO(A-X)
Wavepacket
Rotational
Alignment
Pump/Probe
Photoelectron
Angular
Distribution
Method

48. MISCELLANEOUS

80881. Coplen, T.B., and H.S. Peiser, "History of the Recommended Atomic Weight Values from 1882 to 1997: A Comparison of Differences from Current Values to the Estimated Uncertainties of Earlier Values," *Pure Appl. Chem.* 70, 237-257 (1998).

Atomic Weights
History
Current Values

80882. Wiggins, G., "Chemistry on the Internet: The Library on Your Computer," *J. Chem. Inf. Comput. Sci.* 38, 956-965 (1998).

Internet
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